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Proceedings of the "Science of the Future" Conference – Kazan 2016
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The reports were presented in the following sections:
1. Agricultural, Biological & Food Technologies
2. Chemistry & Chemical technologies
3. Earth Sciences, Ecology & Environmental Management
4. Humanities & Social Sciences
5. Information technologies
6. Life Sciences & Medicine
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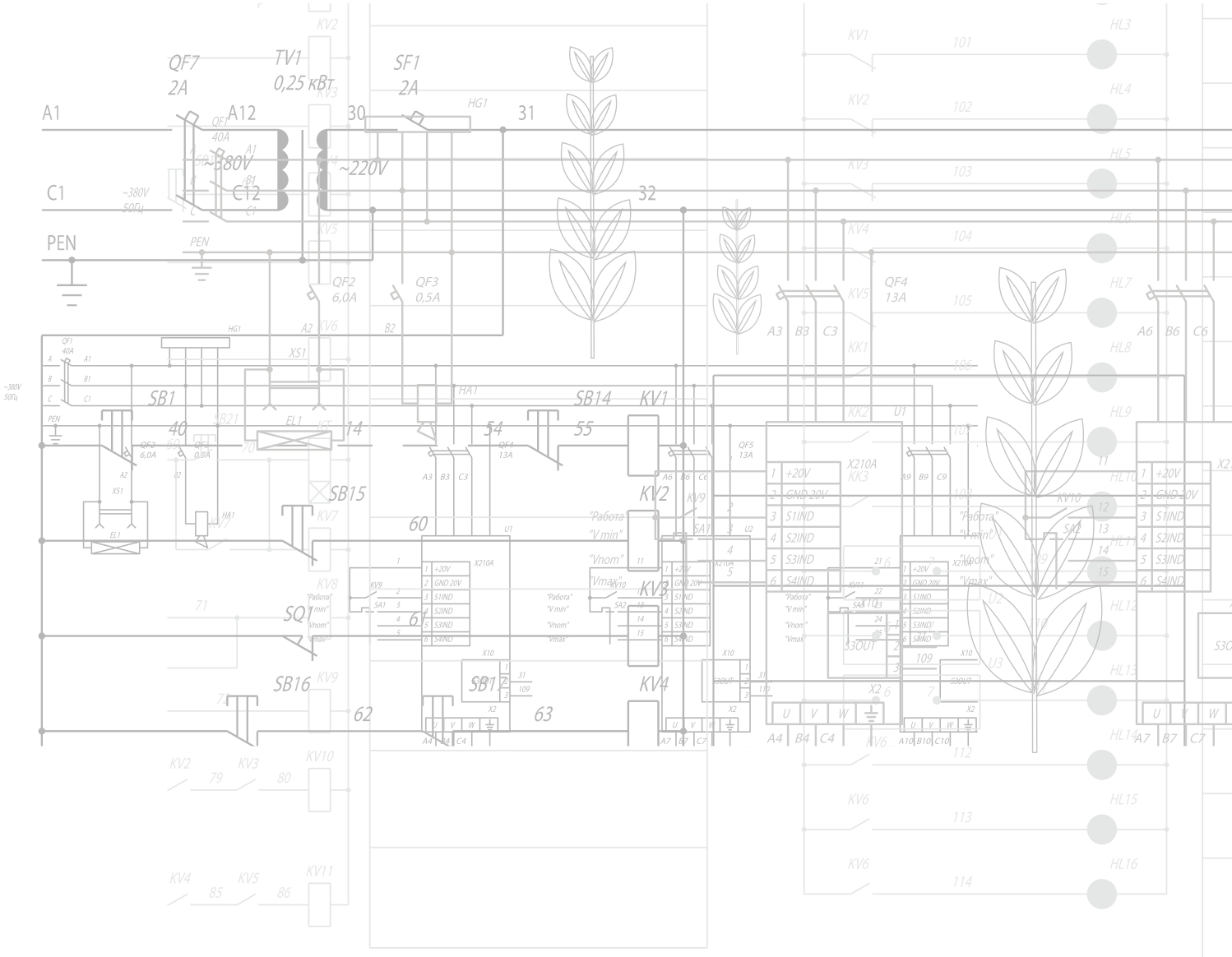
Contents



AGRICULTURAL, BIOLOGICAL & FOOD TECHNOLOGIES

Alekseeva Anastasiya
PhD student

Function of septin proteins in cell division of Drosophila melanogaster S2 cells

SCIENTIFIC ORGANIZATION

Institute of Molecular and Cellular Biology SB RAS and Institute of Chemical Biology and Fundamental Medicine SB RAS

ABSTRACT

Drosophila is a convenient model organism for study septin functions. Here, we investigated the role of all five Drosophila septins in mitosis by their subsequent depletion in cultured S2 cells. We found that depletion of either septin did not affect the mitotic index, although depletion of some septins caused cytokinesis defects. The results suggest the existence of mechanism(s) of interdependent regulation of septins.

KEYWORDS

Septins, cytokinesis, GTPase, cytoskeleton, S2, Drosophila, RNAi.

ACKNOWLEDGEMENTS

We thank L.A. Yarinich (IMCB SB RAS) for RT-qPCR analysis of the RNAi samples.

SUMMARY

INTRODUCTION: Septins are a conserved family of GTP-binding proteins, which were found in all eukaryotic organisms except plants. Numerous studies have shown that these proteins play a key role in carcinogenesis in vertebrates. Septins have the ability to form long filaments, which undergo significant rearrangements during cell cycle, but their functions are not fully understood. The number of septins varies between organisms. For example, in human there are 13 septin genes encoding >30 protein isoforms. Due to the presence of only 5 septins (Sep1, Sep2, Pnut, Sep4 and Sep5), *Drosophila melanogaster* is a convenient model organism for study septin functions. Pnut, Sep1 and Sep2 are known to form heteromeric complex, which can undergo polymerization leading to the formation of filaments. The latter were shown to be involved in the formation of the cleavage furrow during cytokinesis. The function of Sep4 and Sep5 is not yet understood. Here, we studied the role of all five *Drosophila* septins in mitosis by their subsequent depletion by RNAi in cultured S2 cells.

METHODS: Cells were grown in Schneider's medium (Sigma S0146) supplemented with 10% heat-inactivated fetal bovine serum (FBS, Gibco, 10270-106). After 5-day RNAi treatments, cells were fixed and immunostained to reveal microtubules and centrosomes. The following primary and secondary antibodies were used: mouse anti-α-tubulin (Sigma T5168), rabbit anti-DSpd2 [1] (recognize centrosomes), anti-mouse-FITC (Sigma F8264) and anti-rabbit-Alexa568 (Invitrogen A11036). Western-blot and RT-qPCR analyses were employed to assess the efficiency of RNAi. Mitotic index was defined as the percentage ratio between dividing and total numbers of cells in a population.

RESULTS: We found that depletion of either septin did not affect the mitotic index, although depletion of some septins caused cytokinesis defects. Surprisingly, after depletion of some septins we observed altered amounts of transcripts and proteins of some other septins. For example, knockdown of Pnut increased the amount of *Sep4* transcripts and at the same time decreased the amount of *Sep1* and *Sep2* transcripts. The increased amount of *Sep4* transcripts was also detected upon depletion of Sep2, which also caused the decrease of *Sep1* and *pnut* transcripts. Taken together, the obtained results suggest the existence of mechanism(s) of interdependent regulation of septins in cultured *Drosophila* S2 cells.

REFERENCES:

1. M.G. Giansanti et al. (2008) Drosophila SPD-2 is an essential centriole component required for PCM recruitment and astral-microtubule nucleation. Curr. Biol. 18: 303—309.

ADDITIONAL INFORMATION:

A.L. Alekseeva, E.N. Andreyeva, A.V. Pindyurin, S.A. Fedorova

Beckett Richard Peter
PhD
Professor

Extremophile plants: molecular mechanisms of stress tolerance and their practical applications

SCIENTIFIC ORGANIZATION

University of KwaZulu Natal

ABSTRACT

Abiotic stresses, such as drought, salinity, extreme temperatures and chemical toxicity are the primary cause of losses in the majority crops. However, unique “extremophile” plants exist, which can successfully grow in harsh environments worldwide. This talk will review how creating a novel platform based on extremophile plants can lead to new biotechnological approaches for solving problems in agriculture, food production and numerous industrial processes.

KEYWORDS

Stress tolerance, extremophiles, abiotic stress.

SUMMARY

Abiotic stresses, such as drought, salinity, extreme temperatures, chemical toxicity, and prooxidants are serious threats to agriculture and natural ecosystems. Abiotic stress is the primary cause of losses in the majority of wild species and crop worldwide, reducing average yields for most major crop plants by more than 50%. Despite this, unique extremophile plants exist, which can successfully grow in harsh environments. An extremophile (from Latin extremus meaning “extreme” and Greek philiā meaning “love”) is an organism that thrives in extreme conditions that would kill other, less specialized organisms. Among the extremophiles are bryophytes, lichens – symbiotic photosynthesizing organisms, and also some higher vascular plants. Bryophytes and lichens form the dominant plant life over large areas of the world, for example as components of dryland crusts in the steppe, the Arctic, sub-Arctic and Antarctic. To survive in harsh environments, bryophytes and lichens developed tolerance mechanisms to desiccation, high temperature, and low demand for nutrients. We are only beginning to understand their survival mechanisms. One of the factors that determine their high stress tolerance is the presence of redox enzymes with unusual physico-chemical properties. Extremophile plants represent repositories of genes, which with the help of modern technologies can be used to design “super-enzymes” and synthesize “super-metabolites”. The great challenge of modern biotechnology is to develop novel approaches to improving the stress tolerance of non-extremophile plants such as crops using the knowledge of the survival mechanisms of extremophile plants. Furthermore, “extreme” redox enzymes can be an effective instrument in phytoremediation by detoxifying xenobiotics and synthetic dyes and also in industrial processes that require enzymes that can “work” in harsh conditions. The use of enzymes and metabolites derived from extremophile plants represents an ecologically friendly alternative to highly toxic compounds, which are employed for the same purpose at present. This talk will review how creating a novel platform based on extremophile plants can lead to new biotechnological approaches for solving problems in agriculture, food production and numerous industrial processes.

ADDITIONAL INFORMATION

Richard Beckett is Professor of Botany at the School of Life Sciences, University of KwaZulu-Natal, South Africa. He is currently the Academic Leader for Biochemistry, Genetics and Microbiology in his School. Prof Beckett’s research interest is stress physiology of lichens, bryophytes, poikilohydric higher plants and seeds and the biotechnological applications of the enzymes and metabolites of extremophile plants. He has published over 80 research articles, and several major review articles and book chapters. His articles have been cited over 1500 times, and he has a Web of Science “h” score of 23. He is associate editor of the Journal of Bryology and the Lichenologist, the leading journals in his discipline. Prof Beckett has received several grants for international collaboration, including grants from Hungarian, Norwegian, Swedish Foundations, DAAD and DFG, Germany, Leverhulme Foundation, UK, and RFBR, Russia. At present his active international collaborations are with Kazan Institute of Biochemistry and Biophysics, Russia, University of Dresden, Germany, the University of As, Norway, and the University of Innsbruck, Austria.

Krutovsky Konstantin
PhD
Leading Scientist

Pinus sibirica and Larix sibirica whole genome de novo sequencing

SCIENTIFIC ORGANIZATION

Vavilov Institute of General Genetics, Russian Academy of Sciences

ABSTRACT

For the first time the Siberian larch (Larix sibirica) and Siberian stone pine (Pinus sibirica) nuclear and organelle genomes are being de novo sequenced in the Laboratory of Forest Genomics at the Genome Research and Education Center of the Siberian Federal University using Illumina HiSeq 2000 and MiSeq, and their first draft genome assemblies were generated (genome.sfu-kras.ru). About 80% of Siberian larch and pine nuclear genomes consisted of highly repetitive DNA. This study was supported by Research Grant No. 14.Y26.31.0004 from the Government of the Russian Federation.

KEYWORDS

Pinus sibirica, Larix sibirica, genome sequencing, transcriptome, organelle genomes.

ACKNOWLEDGEMENTS

We thank the Siberian Federal University, the Center for Forest Protection in Krasnoyarsk Region, V.N. Sukachev Institute of Forest, Siberian Branch of the Russian Academy of Sciences (SB RAS), Institute of Computational Modeling SB RAS, N.I. Vavilov Institute of General Genetics RAS, Tauber Bioinformatics Research Center, University of Haifa (Israel) and Georg-August University of Göttingen (Germany) for support and Ministry of Science and Education of Russian Federation, Russian Foundation for Basic Research and Russian Government for funding.

SUMMARY

The Siberian larch (*Larix sibirica* Ledeb.) and Siberian pine (*Pinus sibirica* Du Tour.) nuclear and organelle genomes are being *de novo* sequenced in the Laboratory of Forest Genomics at the Genome Research and Education Center of the Siberian Federal University using Illumina HiSeq 2000 and MiSeq, and their first draft genome assemblies were generated (http://genome.sfu-kras.ru/en/main). Estimated genome size was 12.03 Gbp for Siberian larch and 28.90 Gbp for Siberian pine. DNAs isolated from needles, single megagametophytes and a haploid tissue culture of a reference larch tree and from needles and single megagametophytes of a reference pine tree were used to generate multiple PE libraries with 250, 400 and 500 bp long inserts and MPE libraries representing 3 and 5 Kbp long fragments. We tested CLC Assembly Cell, ABySS and MaSuRCA assemblers that were used in the similar conifer genome sequencing projects. The assembling was done using the IBM x3950 x6 server with 96 cores and 3 TB RAM. ABySS was the most stable, but the best assemblies were generated by CLC Assembly Cell. The best Siberian larch genome assembly was ~5.5 Gbp long (that is 46% of the expected complete genome length) with N50 for contigs equaled 1947 bp. Almost all Siberian pine short reads were successfully mapped to the draft genome assembly v1.0 of closely related sugar pine (*Pinus lambertiana* Dougl.) generated in the PineRefSeq project (http://pinegenome.org/pinerefseq) covering more than 80% of the assembly (~21.26 Gbp). Thus, the reference-based together with de novo assembly approaches resulted in a draft genome assembly of Siberian pine with a total length of ~22.9 Gbp (79% of the expected complete genome length) with N50 for contigs equaled 2352 bp. About 80% of Siberian larch and pine nuclear genomes consisted of highly repetitive DNA. For the first time the chloroplast genome of Siberian larch has been assembled and annotated. For Siberian pine we completed the partial chloroplast genome assembly available in Genbank (FJ899558.1) by closing all gaps. The draft assemblies of mitochondrial genomes for these species have been also generated. The larch transcriptome assembly consisted of 43717 unigenes with a total length of ~26 Mbp. The longest unigene was 8512 bp; N50 = 1330 bp, and the number of unigenes longer than 1 Kbp was 6919. The obtained transcriptome assembly was similar to other published conifer transcriptomes. This study was supported by Research Grant No. 14.Y26.31.0004 from the Government of the Russian Federation.

Tikhonovich Igor
Academician
Director of the Institute (ARRIAM)

Role of microbial and plant signals in determination of highly specific symbiosis

SCIENTIFIC ORGANIZATION

All-Russia Research Institute for Agricultural Microbiology, 2.Saint-Petersburg State University

ABSTRACT

Signalling in symbiosis Tikhonovich I.A.1,2, Dolgikh E.A.1, Zhukov V.A.1 1 All-Russia Research Institute for Agricultural Microbiology, Podbelsky chausse 3, 196608, St.-Petersburg, Pushkin, Russia. 2 Saint-Petersburg State University, Universitetskaya emb., 7-9, 199034, St.-Petersburg, Russia. E-mail: ARRIAM2008@yandex.ru Symbiotic receptor kinases play a crucial role in development of legume plants under cooperation with soil microorganisms. Investigation of their structure and functions can help in understanding how plant reacts to environmental conditions.

KEYWORDS

symbiosis, legume plants, nodule bacteria, signalling, Nod factors, microbial colonization, symbiotic receptor kinases

ACKNOWLEDGEMENTS

The research was supported by Russian Science Foundation (grant #16-16-10043)

SUMMARY

Signalling in symbiosis

Tikhonovich I.A.1,2, Dolgikh E.A.1, Zhukov V.A.1

1 All-Russia Research Institute for Agricultural Microbiology, Podbelsky chausse 3, 196608, St.-Petersburg, Pushkin, Russia.

2 Saint-Petersburg State University, Universitetskaya emb., 7-9, 199034, St.-Petersburg, Russia.

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Symbiotic receptor kinases play a crucial role in development of legume plants under cooperation with soil microorganisms. In particular, receptor kinases determine the specificity of interactions with nodule bacteria, take part in signaling during symbiosis development and regulate the intensity of microbial colonization. Investigation of structure and functions of these kinases can help in understanding how plant reacts to environmental conditions, and also can be useful for breeding in conditions of sustainable agriculture.

Specificity of interactions between legume plants and nodule bacteria is based on ligand-receptor interactions, during which the bacterial signal molecules are perceived by plant receptor kinases. Lipochitooligosaccharide signals emanating from rhizobia, known as Nod factors (NFs), trigger a complex of specific responses in the epidermis, pericycle and root cortex of the legume plants, thereby providing the basis for subsequent bacterial entry and organogenesis of root nodules. For many years it has been predicted that legume plants perceive NFs by means of high affinity receptors, triggering signal transduction pathway. Among the evidence is the fact that minor changes in NF structure can change rhizobial host range. Despite some candidate NF receptor genes enconding LysM-receptor-like kinases (LysM-RLKs) have been identified in pea *Pisum sativum*, the underlying mechanisms by which binding of ligand elicits signaling responses remains unclear.

The focus of our research is to unravel these highly specific mechanisms by which rhizobial NFs produced by the symbionts are perceived by the legume plants. To address this aim some new putative LysM-RLKs (K1 and LykX) have been found and characterised in pea. Also the natural polymorphism of these genes was examined in 99 pea genotypes that represent virtually all the diversity within the genus *Pisum*. As a result, it was demonstrated that the allelic state of LykX gene is associated with the ability of plants to form symbiosis with wide spectrum of bacterial strains.

The possible role of new receptors will be discussed. In particular, we propose the model for perception the NF molecule by various receptor complexes.

This study was supported by Russian Science Foundation [grant number 16-16-10043]

Trchounian Armen

PhD., DSc.

Head, Department of Biochemistry, Microbiology and Biotechnology

Biohydrogen and enhancing of its production

SCIENTIFIC ORGANIZATION

Yerevan State University, Yerevan, Armenia

ABSTRACT

Hydrogen (H2) is a clean, effective and renewable fuel which can be produced by different methods including dark and light fermentation by bacteria (biohydrogen) [1]. To develop H2 production biotechnology using of cheap by-products or mixed carbon and utilization of carbon containing wastes, selection of effective bacteria and construction of strains, and optimization of process conditions are reviewed. These approaches could significantly increase H2 production. There are both economic and environmental benefits. [1] A. Trchounian, Crit Rev Biotechnol 35 (2015) 103-113.

KEYWORDS

Biotechnology, Biofuel, Biohydrogen, Bacteria, Fermentation, Wastes.

ACKNOWLEDGEMENTS

Thanks Belgorod State National Research University (Russia) for collaboration.

ADDITIONAL INFORMATION

Corresponding Member of the National Academy of Sciences of Armenia; Laureate of the Prize of the President of Armenia for Development of Natural Sciences; International Association of Hydrogen Energy Akira Mitsui International Awardee for Leadership in Biological Area of Hydrogen Energy.

Vasenev Ivan

Dr.Sc.

Head of Ecology Department

Agroecology-based DSS for Climate-smart farming in the Central Russia conditions

SCIENTIFIC ORGANIZATION

Russian Timiryazev State Agricultural University

ABSTRACT

Modern systems of agroecological monitoring gradually develop the principal information basis for region-adapted DSS on land-use agroecological optimizing. Developed and primary verified in frame of LAMP project (RF Government Grant # 11.G34.31.0079) regionally adapted and climate-smart DSS AKORD-R has framework databases on the actual features of local landscape, soil and soil cover patterns, agroclimate data and agrotechnology parameters, current and previous crops yield, organic and mineral fertilizer doses, technological costs used for profitability analysis.

KEYWORDS

Agroecology, DSS, Climate-smart farming, agroecological modelling, Central Russia.

ACKNOWLEDGEMENTS

Regionally adapted and climate-smart DSS AKORD-R has been developed and primary verified in frame of LAMP project (RF Government Grant # 11.G34.31.0079).

SUMMARY

Aggravating problems of food and environmental security are becoming the key issues of the global challenges of XXI century that was another time declared at the Paris Summit in December 2015. Current models of global changes in XXI century

(IPCC, 2013) show a range of potential global warming from 0.3 (most optimistic version) to more than 4.5 °C at the end of the century, depending on our ability to reduce anthropogenic greenhouse gases emissions. However, at current level of greenhouse gases (GHG) emissions or in case of their future increasing with the same annual rate it is very likely that we will hit the worse case scenarios, with serious negative consequences on environment and more complicated ones on agriculture. For these reasons adaptation to global changes and contributing to climate change mitigation are among the main agroecological challenges addressed to current land-use and land management practice (Foresight, 2011; Beddington et al., 2012; FAO, 2013).

Recently actualized in RF agricultural intensification can essentially increase as GHG emission, including CO_2 (due to non-compensated mineralization of soil organic carbon), CH_4 (fast growing livestock) and N_2O (applying more mineral fertilizers), as carbon sequestration in crop yield and soil organic matter due to more intensive photosynthesis and humification, higher efficiency of fertilizing. Current changes in agroecosystems functioning make important impacts on their farming profitability, regional and global biosphere processes, including C, nutrients' and water balance, climate changes and agroecological potential of adaptation to them. These issues are particularly essential for Central region of Russia, which is characterized by the increased complexity of soil cover due to its comparatively young age, high current spatial differentiation, recent important transformations in land use and agricultural practices.

Modern systems of agroecological monitoring gradually develop the principal information basis for region-adapted decision support systems (DSS) on land-use agroecological optimizing (Vasenev, 2010). Developed and primary verified in frame of LAMP project (RF Government Grant # 11.G34.31.0079) regionally adapted and climate-smart DSS AKORD-R has framework databases on the actual features of local landscape, soil and soil cover patterns, agroclimate data and agrotechnology parameters, current and previous crops yield, organic and mineral fertilizer doses, technological costs used for profitability analysis.

Its region-adapted knowledge base (KnB) allows modeling not only basic agricultural crops yield and their production profitability in concrete landscape and agroclimate conditions, but also evaluate the different agrotechnologies efficiency for various scenarios of climate change. Climate-smart module of AKORD-R KnB is based on last techniques of the EU, summarized in "Climate Smart Agriculture" (FAO, 2013), after their adaptation to the climatic and soil-geomorphological conditions, land-use structure, and dominating agrotechnologies at the Central part of European Russia.

Together with the regional/ local systems of agroecological zoning, degradation risk and land quality assessment scales, crop (variety) and agrotechnology requirements, the previous farming practices results they allow to develop spatial and temporally differentiated most probable agroclimatic predictions and crop production models, the region-adapted framework systems of land agroecological functions, algorithms and standard data for their evaluation.

Sustainable climate-smart farming refers to the flexible balance among its land principal agroecological functions in changing landscape and agricultural conditions:

1. Agroclimatic function of plant supply with photosynthetic active radiation, effective heat and available moisture;
2. Agrochemical function of crop supply with available macro- and micro-nutrients;
3. Agrophysical function of favorable condition support for effective work of the agricultural machines;
4. Hydrophysical function of plant seasonal supply with available moisture and soil air exchange;
5. Phyto-sanitary function of favorable condition support for crop without damage by pathogens, pests and weeds;
6. Ecogeochemical function of land resistance to contamination;
7. Ecopedomorphogenetic function of plant and farming support with soil-ecological condition quasi-homogeneity in space and time.

DSS AKORD-R includes the integral land evaluation algorithm consisted from four special modules. Primary algorithm (parametric analysis) describes the principal

agroecological parameters assessment by their modelling or adapted to concrete soil and agricultural land type logistic equation. Second one (factor analysis) includes each agroecological function assessment as corrected harmonic mean from its parameters assessment values. Third algorithm (land analysis) determines homogeneous land unit assessment as combination of its functions values. Fourth one (field analysis) runs the heterogeneous land unit assessment as weighted average value corrected by soil cover patterns contrast and boundary complexity.

Its application is very useful for fast decision on new fields' choice for most profitable crops in fast changing market, technology, climate and weather conditions. The same it is necessary to apply this tool for land agroecological typification and best available farming technologies transfer.

AKORD-R crop selection module include submodules on landscape (meso- and micro-relief, parent materials, ground water) ecological limiting factor assessment, predecessor set aftereffect analysis, predicted yield and scheduled costs evaluation.

Complex module of crop production modeling runs through PAR-based yield evaluation and analysis its limitation by inefficient soil available water supply or precipitation levels, soil macro- and micro-nutrients content or adverse acid-base conditions, unfavorable soil bulk density or phyto-sanitary state. PAR-based yield evaluation algorithm takes into consideration the vegetation period duration and its seasonal distribution, site geographical coordinates and its PAR value according to regional agroclimatic GIS, slope exposure and gradient, crop and variety features. Precipitation various predictions are based on their perennial statistics and global-change trends. Seasonal soil available water supply (SAWS) prediction takes into consideration not only seasonal precipitation, but also the previous fall characteristics and/or spring SAWS, the same as topsoil texture, structure, crop and slope parameters that determine soil infiltration rate and run-off in different precipitation and vegetation conditions.

Climate-smart module allows predicting crop development and yield in concrete land and various agro-climate and technology conditions for best available farming practice selection with minimum environmental and economic risks. Principal tasks of environmentally friendly and climate-smart land-use annual correction usually include the following target issues:

- Effective increase in production level and land-use efficiency (productivity/profitability),
- Improvement of consumer, technological and ecological quality of the end production (for example, increase in the content of protein or starch),
- Seasonal expansion and/or redistribution of the arable lands for different crops due to market needs dynamics,
- Agrotechnology adaptation to the current agrolandscape conditions, in particular connected with local climate change and/or forecrop impacts,
- Agroecologically based agrotechnology transfer through its consequences modelling, verification and adaptation to concrete regional and agrolandscape features,
- Support for production and farming system ecological certification,
- Prevention or minimizing the negative economic consequences of the drought, erosion, leaching and other problem agroecological situation development due to long-term farming practice and global changes.

Adapted to Central region of Russia climate-smart DSS AKORD-R is becoming the convenient framework tools for environmentally friendly and climate-smart agricultural land-use design taking into attention the regional and landscape-based features of the concrete soil cover patterns, land-use history, planned crops, farming subsystems and best available technologies, adapted to local agrolandscape conditions.

Vasyutinskii Oleg
Doctor of Sciences
Leading Researcher

Laser methods for modern biotechnologies

SCIENTIFIC ORGANIZATION

Ioffe Physical-Technical Institute of the Russian Academy of Sciences, St.Petersburg

ABSTRACT

The talk presents results obtained at Ioffe Institute on laser methods applied for modern biotechnologies and a proposal based on state-of-the-art laser methods and aimed to address several important problems in four closely interwoven research directions at the interface of chemistry, biology, physics, and medicine: (1) real time energy transfer in biologically relevant molecules; (2) decomposition of amino acids isolated in a supersonic molecular beam; (3) live cells and cellular structures morphology and dynamics; (4) quantum magnetic sensors for bio-structure analysis.

KEYWORDS

Laser technologies, multiphoton transitions, digital holographic microscopy, cellular structure and dynamics, photodynamic therapy, cancer diagnostics, biomolecule radiation stability, magnetic properties of biostructures.

Velikova Dimitrova Svetla
M.D., Ph.D
Expert

Boosting the cognitive functions according to the personal EEG profile

SCIENTIFIC ORGANIZATION

European Commission, Brussels, Belgium

ABSTRACT

The presentation discuss the use of quantitative electroencephalography (EEG) for obtaining individual 'portrait' of brain functioning and how this information can be used for personalized enhancement of cognitive abilities with non-invasive solutions, especially neurofeedbeck.

KEYWORDS

Cognition, EEG, neurointerface.

SUMMARY

With the high level of dynamics and competition today many people encounter the necessity to optimize their cognitive performance, and there appear two questions: how to chose the most effective approach that at the same time is healthy? The problem is very complex and unfortunately there is not a unique recipe for everybody. But how the neuroscience can help us to find the best individual solution? The first step is to define the current needs, according to that how our brain is performing and an important help can be obtained by application of electroencephalographic approach (EEG). The quantitative EEG (QEEG) allows to obtain very detailed information about the brain functioning during resting state or during performance of different tasks. It is established that the brain map of a certain individual is like a fingerprint – the personal EEG is relatively stable with the years and therefore in some sense "typical" for a person. When many EEG parameters are considered, the EEG maps of different people show enormous variety. The EEG maps of persons with equal (according to the psychological tests) cognitive abilities can look very different, because beside of a certain common used psychometric term, like for example the attention, from psychophysiological (i.e. QEEG) point of view can be distinguished and assessed many different oscillatory processes having contribution to the process of 'attention'. Consequently, combining psychological testing with QEEG gives several advantages, since the QEEG can be very precise in giving information 'what exactly happens' from functional point of view and eventually at which stage of a certain process the person encounter some problems. Such a detailed report about the different level of the functioning

in the brain linked with a certain psychometric parameter, allows further to the plan individual interventions in order to modify brain activity and finally enhance the individual performance. A widely used non-invasive approach for boosting cognitive performance is the neurofeedbeck. An important advantage of the intervention is that it is non-invasive and safe. The QEEG can act as a navigator for planning the parameters and sequence of neurofeedbeck procedures and therefore to provide maximum tailored training of the brain functions.

With the development of neurointerfaces for home use, providing options for personalized optimization of cognitive functioning appears the next challenge for the neuroscientists.

Zaitsev Sergey

Doctor of Science degree in biochemistry

Head of the Chemistry Department of the Moscow SAVMB

Dynamic surface tension measurements as general approach to the analysis of animal blood plasma and serum

SCIENTIFIC ORGANIZATION

Federal State Budgetary Educational Institution of Higher Education “Moscow state Academy of Veterinary Medicine and Biotechnology - MVA by K.I. Skryabin”

ABSTRACT

This report summarizes a current state of knowledge regarding surface tension methods of the analysis of animal blood plasma and serum as the major biological liquids. The fundamental information on general properties of the biological liquids (animal blood, urea, milk, etc.) is important in many aspects: animal nutrition, health assessment, physiological control, quality of livestock production, etc. The comparison of the major methods of the static and dynamic surface tension (DST) measurements of various liquids is presented. The comprehensive analysis of some colloid properties of animal biological liquids, including the study of the DST parameters (surface tension values at particular time intervals, tilts of the tensiograms) and the protein–lipid–salt content, is proposed. Strong or medium positive (negative) correlations between DST and biochemical parameters (content of total and particular proteins, lipids, etc.) are obtained and discussed for a few animal groups (fillies, mares, stallions, bulls, heifers, pregnant and lactating cows) for the first time. The data obtained highlight the importance of the particular balances and vital functions of the main components in such an important biological liquid as blood plasma. The reliability of the correlations between the DST and the biochemical parameters of animal blood samples under normal and particular physiological conditions (age, gender, pregnancy, lactation period, etc.) is shown. The database of the DST values will be useful in fundamental areas (colloid and physical chemistry, bioorganic and biological chemistry, animal biology, and ecology), as well as in practice (animal medicine and biotechnology, dairy and meat production, etc.).

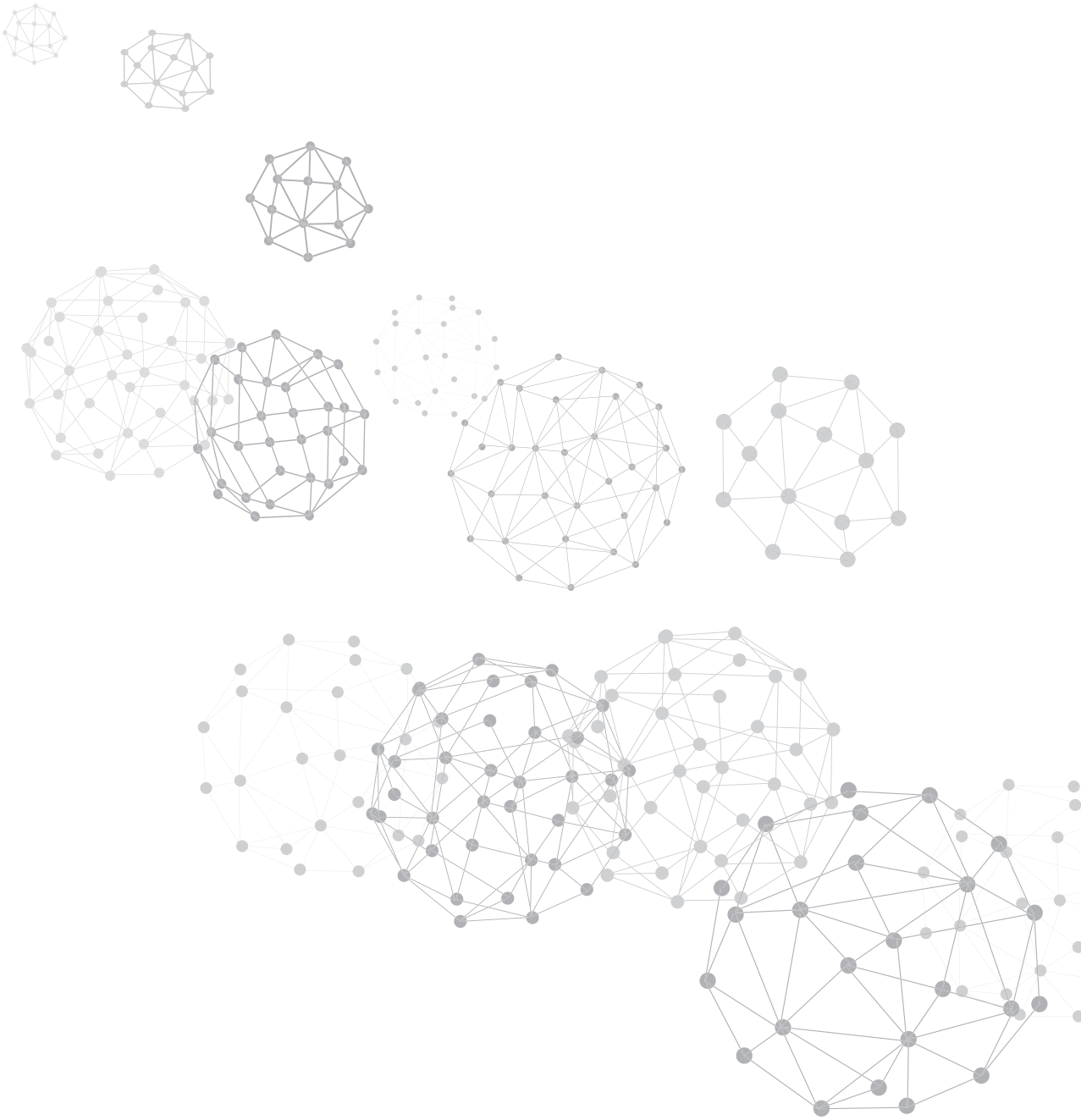
KEYWORDS

* Scientific discipline * animal biochemistry, blood, milk, biocolloids, supramolecular systems, surface tension methods, correlations.

ACKNOWLEDGEMENTS

The study was supported by the grant from the Russian Science Foundation (project no. 14-16-00046).

Advances in Colloid and Interface Science 235 (2016) 201–213 http://dx.doi.org/10.1016/j.cis.2016.06.007



CHEMISTRY & CHEMICAL TECHNOLOGIES

Akhmetshina Tatiana
Laboratory assistant

The nanocluster analysis of intermetallics: the collection of Topological Types of Nanoclusters (TTN) and its application

SCIENTIFIC ORGANIZATION

Samara National Research University

ABSTRACT

Using the ToposPro program package we have created the Topological Types of Nanoclusters (TTN) collection, which contains information on more than 2000 structural building units. We have shown the possibilities of the TTN collection by analysis of icosahedron-, Bergman-cluster and Mackay-cluster-based intermetallics. The chemical composition of the nanoclusters and topological parametres were considered and correlations between them were found. In the future the TTN collection will be transformed into a knowledge database of an expert system.

KEYWORDS

Intermetallics; nanocluster analysis; clusters; databases; expert systems.

ACKNOWLEDGEMENTS

The authors are grateful to the Russian Government (Grant 14.B25.31.0005) for support.

SUMMARY

Using the data on more than 27,000 crystal structures of intermetallics from the ICSD and Pearson's Crystal Data and the ToposPro program package [1] we have created the *Topological Types of Nanoclusters* (TTN) collection, which contains information on the structural building units. The TTN collection contains 1006 polyhedral and 1016 multishell nanoclusters as local configurations of atoms and as primary nanoclusters in intermetallics. We have shown the possibilities of the TTN collection by analysis of icosahedron-, Bergman-cluster and Mackay-cluster-based intermetallics. These clusters are chosen as the most fascinating and frequently encountered structural units in intermetallic compounds. To analyze these structures, we have applied a universal method based on the strict algorithm of searching for the multi-shell onion-like primary nanoclusters that assemble the intermetallic structures [2]. We have considered the chemical composition of the nanoclusters as well as the ways of their local and overall binding. As a result, we have found correlation between chemical composition and topological parameters, which could be very useful for prediction of new intermetallic compounds. For instance, if the inner icosahedron of a Mackay nanocluster consists of the same atoms and composition of the second shell is 30A+12B, the topology of underlying net is body-centered cubic (**bcu-x**) in 82% cases. Another example concerns icosahedron-based intermetallics: the A@M12 composition is realized in 87 compounds out of which 84 structures are assembled in accordance with the **bcu-x** motif. In the future we are going to include the information about the distributions of the topological parameters and their correlations to the TTN collection and transform it to a knowledge database of an expert system.

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ADDITIONAL INFORMATION

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Knowledge-based approach for prediction of 2D coordination polymers exfoliation

SCIENTIFIC ORGANIZATION

Samara Center for Theoretical Materials Science, Samara National Research University

ABSTRACT

We generalized the accumulated data for exfoliated 2D coordination polymers to reveal the main structural features leading to easy exfoliating materials, and to elaborate recommendations for using this technique. In our study, we used abilities of programs for crystallochemical analysis to find correlations between structural descriptors of bulk materials, conditions for exfoliation, and parameters of nanomaterials. Using knowledge-based approach, we selected six coordination polymers for experimental check of revealed recommendations.

KEYWORDS

Knowledge-based approach, 2D coordination polymers, exfoliation, nanosheets.

ACKNOWLEDGEMENTS

E.V.A. thanks the Russian government (grant No. 14.B25.31.0005), Russian Foundation for Basic Research (grant No. 16-37-00147), and Russian Ministry of Science and Education for support.

SUMMARY

The idea of coordination polymers (CPs) nanosheets study originates from successful delamination of graphene [1] and other numerous layered inorganic materials. 2D CPs nanosheets have advantage in comparison to this materials due to a variability of composition (almost infinite combinations of metals and ligands), structures (more than 2000 topological types and 20000 structures [2, 3]), and promising properties (electric, magnetic, optical, sieving, catalytic, drug delivery etc. [4]). Despite the fact, in one of the first reviews about 2D polymers nanosheets the coordination polymers were considered as “to be unlikely that they will be separable from one another” [5], the 2D coordination polymer [Zn(adc)] (adc= adamantane-1,3-dicarboxylate dianion) was exfoliated at first time in 2008 [6]. In general, there were 18 publications about exfoliation of 33 2D CPs, which discussed in 11 reviews. However, these works concern only properties of obtained nanomaterials without formulating any generalized concept or strategy for selecting bulk materials and conditions for exfoliation. All experiments were based on serendipity of scientists.

We tried to generalize the accumulated data for exfoliated 2D CPs materials. The special attention was paid to crystallochemical characteristics of the structures with goal to reveal the main principles for finding materials and appropriate exfoliation techniques. Thus, solvent selection is not trivial. Indeed, it should correlate to structural characteristics of sample. The adjustment of sonication parameters (power and time) has influence in thickness and lateral dimension of the nanosheets. However, the main problem is to find the appropriate conditions to get either single layers or few layers, but with large enough lateral dimensions in comparison to the thickness [7]. In our study, we used abilities of program packages for crystallochemical analysis (ToposPro [8], Platon [9] etc.) to find relations between structural descriptors of bulk materials (composition, structural units, single layer topology, charge, thickness, geometry, intra- and interlayer interactions, interlayer distance, porosity) and exfoliation parameters of nanomaterials (stability, solvent, mechanical treatment, dimensions and shape of nanoparticles).

It was found, that the structures containing polar structural groups (-CO, -SO, -PO, -NH, -OH, -Cl) on the surface can be easily exfoliated in polar solvents (H_2O, EtOH), and more hydrophobic solvents (DMF, toluene) are preferable for layers with less polar surface (-CH). The size of solvent molecules plays decisive role for exfoliation: small molecules more frequently and successfully leads to exfoliation. Strong interlayer interactions prevent exfoliation with simple solvent technique, the use of surfactant is necessary. Porous structures containing intercalated solvent molecules can be exfoliated with more probability.

In general, two hypothetical models for exfoliation mechanism were proposed:

1. Swelling the porous structure by solvent and subsequent separation of solvated nanosheets.
2. Delamination of nanosheets starting from breaking of interlayer interactions from crystal faces and diffusion of solvents into interlayer space.

Revealed correlations were used for selection of six 2D CPs from CSD [10] and subsequent exfoliation in water, ethanol, acetone, and THF. These bulk materials satisfied to the following recommended criteria:

1. Flat layers with large interlayer distances or pores.
2. Polar groups on the layer surface are able to contact with solvent molecules.
3. Only weak van der Waals' interactions between layers.
4. Coordination bonds are strong enough to stabilize nanosheets.

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Converting Solar Energy into Storable Fuels: Understanding the Chemistry of the Underlying Photocatalytic Processes

SCIENTIFIC ORGANIZATION

Saint-Petersburg State University

ABSTRACT

Photoelectrochemical and Photocatalytic Processes are ideally suited for direct conversion of Solar Energy into Storable Chemical Fuels. The reported efficiencies are very low. Any enhancement of the efficiency of the utilization of photogenerated charge carriers on the surface of photocatalysts requires an enhanced understanding of the entire photocatalytic process. This lecture provides some necessary tools for the understanding and the development of the photocatalytic reaction mechanism with the aim to improve the conversion efficiency of solar into chemical energy.

KEYWORDS

Photoelectrochemical and Photocatalytic Processes, Solar Energy, Storable Fuels.

ACKNOWLEDGEMENTS

The present study was performed within the Project "Establishment of the Laboratory "Photoactive Nanocomposite Materials" No. 14.Z50.31.0016 supported by a Mega-grant of the Government of the Russian Federation.

SUMMARY

Photoelectrochemical and Photocatalytic Processes are, in principle, ideally suited for the direct conversion of Solar Energy into Storable Chemical Fuels. However, the reported efficiencies of the overall as well as of the individual reduction and oxidation processes are still very low, often below 1 %. Any enhancement of the efficiency of the utilization of photogenerated charge carriers on the surface of photocatalysts requires an enhanced understanding of the entire photocatalytic process. The reduction potentials of most substrates, as well as those of the intermediates formed during the photocatalytic reaction(s), are well known; nevertheless, it is essential to realize that thermodynamic properties may change upon the adsorption of these molecules at the photocatalyst surface. Therefore, a detailed understanding of the processes occurring on the photocatalyst surface before, during, and after light absorption is of utmost importance. On the other hand, the charge carriers generated upon light absorption that survive recombination and reach the semiconductor surface may suffer surface recombination processes or recombination via an electron shuttle mechanism (Z scheme deactivation mechanism), thus reducing the total efficiency of the photocatalytic system. Moreover, since the overall efficiency of a photocatalytic process will be determined by the efficiency of the slowest reaction step it is crucial to know whether this is the reductive or oxidative half-reactions. Besides the obvious one-electron transfer steps these reactions entail in particular multi-electron transfer processes, e.g., the four-electron oxidation of water or the eight-electron reduction of CO_2. Hence, this lecture provides some necessary tools for the understanding and the development of the photocatalytic reaction mechanism with the aim to improve the conversion efficiency of solar into chemical energy.

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Topological approaches to design of new materials

SCIENTIFIC ORGANIZATION

Samara National Research University

ABSTRACT

We present new concepts, descriptors, methods, software, and databases, which we have developed for the topological analysis and design of new substances and materials. We consider our development of hybrid methods for designing structure of substances and materials. These methods include fast screening of topological knowledge bases for a qualitative or semi-quantitative prediction and subsequent precise estimation of physical properties of the substance by mathematical modeling (DFT or molecular dynamics).

KEYWORDS

Materials science; topological methods; knowledge databases; design; DFT; hybrid methods.

ACKNOWLEDGEMENTS

This work was supported by the Government of the Russian Federation (project 14.B25.31.0005)

SUMMARY

Analysis of topological properties of crystal structures becomes more and more widespread; we can state that a new branch of science, topological crystal chemistry, has been formed. Here we present new concepts, descriptors, methods, software, and databases, which we have developed for the topological analysis and design of new substances and materials.

We have created knowledge databases containing correlations ‘chemical composition - local topology of complex groups - overall topology of coordination polymer’. Such databases help one to predict the connectivity of structural units (complexing atoms, ligands, clusters and polynuclear complex groups), the resulting topology of the polymeric motifs, and the probability of formation of the corresponding architectures.

We discuss examples of application of the topological approaches to the analysis of molecular packing, modeling of microporous frameworks, prediction of ionic conductivity in inorganic ionic substances, nanocluster modeling of intermetallic compounds.

We consider our development of hybrid methods for designing structure of substances and materials. These methods include fast screening of topological knowledge bases for a qualitative or semi-quantitative prediction and subsequent precise estimation of physical properties of the substance by mathematical modeling (DFT or molecular dynamics). As a result, the number of models to be considered in the simulation sharply reduces, and design of new compounds significantly accelerates.

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Polymeric Nanocarriers for Targeted Drug Delivery

SCIENTIFIC ORGANIZATION

University of Nebraska Medical Center

ABSTRACT

Nanoscale polymeric particles, in particular self-assembled block copolymer micelles, have been utilized in pharmaceutics for development of novel therapeutic and diagnostic modalities. They can be designed to facilitate the incorporation of a variety of compounds or even particles through a combination of electrostatic, hydrophobic, and hydrogen bonding interactions. The potential application of such polymeric micelles as carriers for multidrug delivery will be discussed.

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Shaping of sulfated zirconia oxide catalyst and its impact on physico-chemical properties and activity in model reactions of n-hexane isomeriation and isobutane alkylation

SCIENTIFIC ORGANIZATION

St. Petersburg State Technological Institute (technical university)

ABSTRACT

Sulfated zirconium hydroxide shaping by extrusion is studied based on elucidating impact of zeta-potential and rheological characteristics on physical and chemical properties of technical catalysts. The pore structure of shaped catalysts was unaffected by rheological parameters. At the same time deviations of the zeta potential from the zero-value afforded more uniform pore structure. Shaped at various zeta-potential values catalysts demonstrated different activity in model reactions of isobutane alkylation and n-hexane isomerization.

KEYWORDS

Sulfated zirconia, shaping, zeta-potential, alkylation, isomerization.

ACKNOWLEDGEMENTS

The work was performed as part of the state contract awarded on the basis of a grant of the Government of the Russian Federation for support of scientific research conducted under the supervision of leading scientists at Russian institutions of higher education, research institutions of State Academies of Sciences and state research centres of the Russian Federation on March 19, 2014, no. 14.Z50.31.0013.

SUMMARY

The present work focuses on investigation of such important catalyst material as sulfated zirconia, which is used in a number of acid-catalyzed chemical reactions including alkylation of isobutane and isomerazation of paraffins practiced on industrial level. In the current work sulfated zirconia catalyst shaping process is discussed from the viewpoint of rheology. In more detail an influence of zeta-potential

(charge near to particle's surface), polyvinylalcohol (PVA) addition and alumina binder content on the mechanical strength, surface acidity and textural characteristics is addressed. Model reactions of isobutane alkylation and n-hexane isomerization were chosen to relate influence of shaping parameters on catalysts' activity.

According to zeta-potential titration measurements of sulfated zirconium hydroxide with PVA additions, the latter is considered as a weak surface-modifying agent. It slightly shifts point of zero charge of particles. Although rheological measurements demonstrated decrease of the yield stress while introducing PVA, as a result from water-polymer interactions thus leading to more prominent slipping of particles in the suspension. However, it was shown that PVA does not modify acidity, surface area or mechanical strength of final catalysts; consequently, it could be used just as an extrusion aid.

The Krieger-Dougherty model was used to fit the experimental data of the dependence of apparent viscosity on suspensions' solid fraction. Fitted shape-factor constant was very close to the one for the spherical monodisperse particles, what is also confirmed by SEM study.

As a consequence of the fact that sulfated zirconium hydroxide cannot be shaped alone, its colloidal properties was also studied in the presence of boehmite binder. Zeta-potential titration curves demonstrated that there is an interaction between aluminum species and zirconium ones. Fitting rheological data to Krieger-Dougherty equation showed that boehmite and sulfated zirconia hydroxide tends to form secondary aggregated structures.

Choose of zeta-potential value during shaping process influences on pore-size-distribution curves of the final catalysts and crushing strength. Also, it can slightly modify catalysts' acidity, what can be explained through migration of alumina species on zirconia surface.

Deconvolution results of pore size distribution curves can distinct the presence of two peaks, which are attributed to zirconia and alumina structures. Choose of zeta-potential value during shaping results in the relative changes of the two peaks areas. At higher values of zeta-potential, uniform structure is formed, while at low values bimodal one was obtained.

Catalytic measurements using model reactions showed that catalysts' shaping parameters have a strong impact on its activity. Thus, catalyst's scale-up from laboratory level to industrial should be done with great care and account for structure's and active center's changes during production process.

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Magnetic field-sensitive carriers for biomolecules immobilization on the basis of magnetite-gold hybrid nanoparticles

SCIENTIFIC ORGANIZATION

Lomonosov Moscow State University

ABSTRACT

During last decades magnetite nanoparticles (NPs) attract a deep interest of scientists due to their potential application in therapy and diagnostics. However, magnetite nanoparticles are toxic and non-stable in physiological conditions. To solve these problems, we decided to create two types of hybrid systems based on magnetite and gold which is inert and biocompatible: gold as a shell material (first type) and gold as separate NPs interfacially bond to magnetite NPs (second type).

KEYWORDS

Regulation of enzyme activity, drug delivery, magnetite-gold nanoparticles.

ACKNOWLEDGEMENTS

This work was supported by Grant of Russian Scientific Foundation 14-13-00731, Grant of Ministry of Education and Science of the Russian Federation (14.607.21.0132, RFMEFI60715X0132) and MSU development program 5.13.

SUMMARY

The synthesis of the first type hybrid nanoparticles was carried out as follows: magnetite nanoparticles with an average diameter of 9±2 nm were obtained by co-precipitation of iron (II, III) chlorides then they were covered with gold shell by iterative reduction of hydrogen tetrachloroaurate with hydroxylamine hydrochloride. According to the TEM, ICP MS and EDX data, final nanoparticles had an average diameter of 31±4 nm and contained iron even after hydrochloric acid treatment. However, iron signals (K-line, 7,1 keV) were not localized so we can't speak about one single magnetic core. Described nanoparticles covered with mercapto-PEG acid were non-toxic for human prostate cancer PC-3/ LNCaP cell lines (more than 90% survived cells as compared to control) and had high R2-relaxivity rates (>190 mM-1s-1) that exceed the transverse relaxation rate of commercial MRI-contrasting agents. These nanoparticles were also used for chymotrypsin enzyme immobilization. The effect of alternating magnetic field on catalytic properties of chymotrypsin immobilized on magnetite nanoparticles, notably the slowdown of catalyzed reaction at the level of 35-40 % was found. The most probable reason for the observed effect is the change of active centers topology on the enzyme surface as a result of its deformation under applied forces.

The synthesis of the second type hybrid nanoparticles also involved two steps. Firstly, spherical gold nanoparticles with an average diameter of 9±2 nm were synthesized by the reduction of hydrogen tetrachloroaurate with oleylamine; secondly, they were used as seeds during magnetite synthesis by thermal decomposition of iron pentacarbonyl in octadecene. As a result, so-called dumbbell-like structures were obtained where magnetite (cubes with 25±6 nm diagonal) and gold nanoparticles were connected together pairwise. By HRTEM method (first time for this type of structure) an epitaxial growth of magnetite nanoparticles on gold surface with co-orientation of (111) planes was discovered. These nanoparticles were transferred into water by means of block-copolymer Pluronic F127 then loaded with anti-cancer drug doxorubicin and also PSMA-vector specific for LNCaP cell line. Obtained nanoparticles were found to have moderate toxicity for human prostate cancer cells and got into the intracellular space after 45 minutes of incubation (according to fluorescence microscopy data). These materials are also perspective from MRI point of view (R2-relaxivity rates >70 mM-1s-1).

Thereby, in this work magnetite-gold hybrid nanoparticles, which have a strong potential for biomedical application, particularly in targeted drug delivery and magnetic resonance imaging, were synthesized and characterized. That paves the way to the development of new medicine types – theranostics.

ADDITIONAL INFORMATION

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Advances in new generation photoactive materials

SCIENTIFIC ORGANIZATION

Saint-Petersburg State University

ABSTRACT

A review of the concept and recent advances in the studies related to the third generation of photoactive materials performed in the Laboratory "Photoactive Nanocomposite Materials" of SPbSU is given. The major attention is focused on the heterostructured materials realizing Z-scheme of two-photon excitation and charge separation, enhancement of the surface activity due to the effect of the localized surface plasmon resonance, and application of up-conversion materials to achieve higher spectral sensitivity of hybrid photoactive materials.

KEYWORDS

Photoactive materials, photocatalysis, solar energy conversion, localized surface plasmon resonance, Z-scheme, up-conversion.

ACKNOWLEDGEMENTS

The present study was performed within the Project "Establishment of the Laboratory "Photoactive Nanocomposite Materials" No. 14.Z50.31.0016 supported by grant of the Government of the Russian Federation. The authors are also grateful to Research Park at the Saint-Petersburg State University for the technical support.

SUMMARY

To overcome three major challenges existing for photoactive materials: higher activity, higher sensitivity to the visible light, and higher selectivity in heterogeneous photoreactions, a new concept of the third generation of photoactive materials has been considered recently [1]. The concept is based on the nanoconstruction of heterostructured materials as a combination of materials with different properties that results in improvement of the functional characteristics of the nanocomposite materials and enhancement of required reaction pathways comparing to the side processes. In this presentation a review of the concept and recent advances in the studies related to the third generation of photoactive materials performed in the Laboratory "Photoactive Nanocomposite Materials" of SPbSU and elsewhere in the world is given. The major attention focuses on the heterostructured materials realizing Z-scheme of two-photon excitation and charge separation, enhancement of the surface activity due to the effect of the surface localized plasmon resonance, and application of up-conversion materials to achieve higher spectral sensitivity of hybrid photoactive materials.

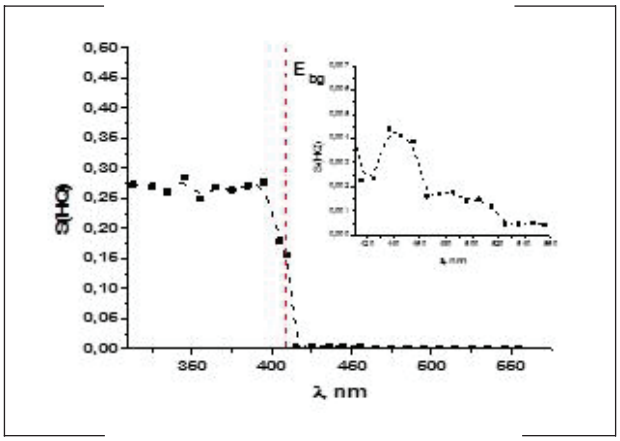
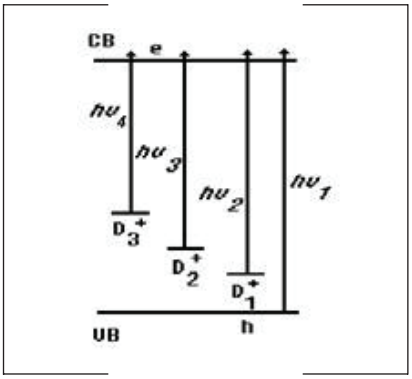


Fig. 1 Spectral dependence of the Pt-TiO_2 selectivity toward formation of hydroquinone during phenol photodegradation.

Fig. 2. Mechanism of photoexcitation of doped photoactive materials resulting in the spectral selectivity.



Second generation photoactive materials

The major advantages achieved with the second generation photoactive materials produced by either metal or non-metal doping and co-doping, is an extension of the spectral range of the surface photochemical activity toward visible light. As demonstrated by spectral dependences of the surface selectivity (see Fig. 1), this extension is due to formation of the localized electronic states, which photoexcitation results in generation of the different types of the surface active centers (see Fig. 2).

Thus, purposeful alteration of photoexcitation mechanism of such materials should result in alteration of the activity and selectivity of photoactive materials. This alteration is a distinguishable feature of the new generation materials. It can be achieved by formation of multi-component heterostructures.

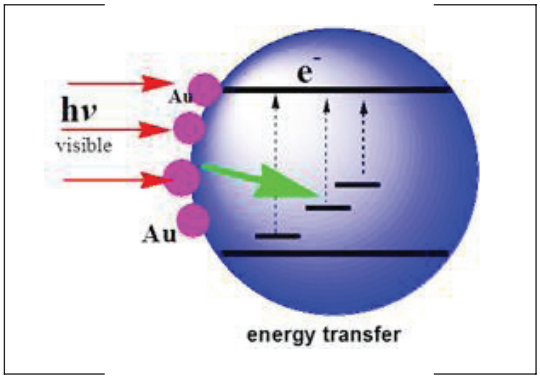


Fig. 3 Mechanism of energy transfer from plasmonic metal states to electronic states in semiconductor.

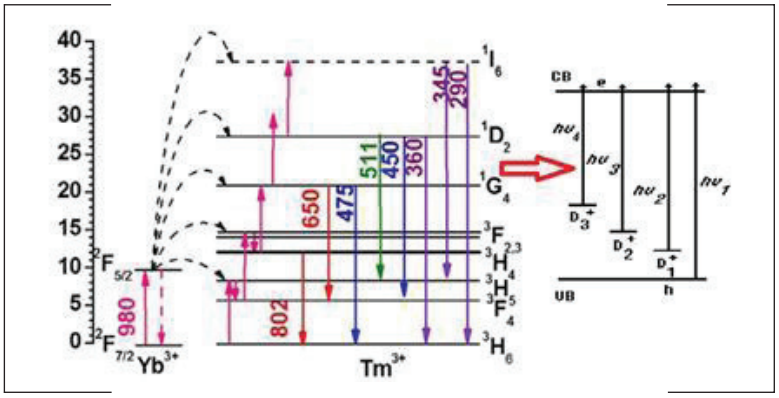


Fig. 4 Mechanism of energy transfer from up-converter states to electronic states in semiconductor.

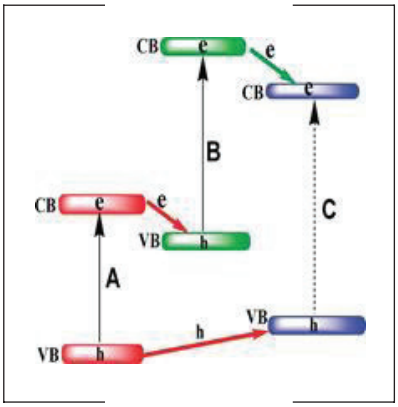


Fig. 5. Z-scheme oft wo-photon excitation and charge separation in heterostructured materials.

Surface localized plasmon resonance (SLPR)

The distinguished features of the SLPR effect is the are the dependence of the position of the resonance absorption band on the size and shape of the metal nanoparticles and redistribution of the electromagnetic field around the metal particles. In other word, the metal nanoparticle serves as an wavelength selective antenna and energy re-transmitter. This phenomenon allows selectively to enhance the excitation of electronic states in photoactive semiconductor materials (see Fig. 2) as a component of the heterostructured new generation materials, due to near-resonance energy transfer (see Fig. 3).

Thus, the SLPR effect can tune and enhance visible light activity and selectivity of photoactive materials.

The summary of the recent results related to the application of SLRP effect in new generation photoactive materials obtained in the Laboratory “Photoactive Nanocomposite Materials” of SPbSU and elsewhere will be given during presentation.

Up-conversion

The effect of up-conversion provides the ability to utilize IR-light to reach the excited states that otherwise correspond to photoexcitation with either visible or UV-light due to energy transfer processes in up-converters (see Fig 4). The possibility of energy transfer from the up-converter component to semiconductor in hybrid heterostructured photoactive materials provides the condition for excitation of the semiconductor component to initiate surface chemical sequences.

Manipulation with the concentration of active elements in up-converters allows to tune the transferred energy and therefore, provides the conditions for selective tuning and enhancement of the activity and selectivity of semiconductor surface.

The summary of the recent results related to the application of up-conversion effect for photoexcitation of new generation photoactive materials obtained in the Laboratory “Photoactive Nanocomposite Materials” of SPbSU and elsewhere will be given during presentation.

Z-scheme of photoexcitation

The problem of the spectral sensitization of wide band gap semiconductors and enhancment of their activity through the effective charge separation can be solved by application of the concept of heterostructured materials realizing so called Z-scheme of multi-photon excitation and charge separation at heterojunctions (see Fig. 5).

One of the promising systems with proper position of the energy states of the components can be the heterostructure $TiO_2/WO_3/CdS/TiO_2$. The summary of the recent results related to the application of Z-scheme mechanism in new generation photoactive materials for photoelectrochemistry and photocatalysis will be given during presentation.

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Chain coordination polymers: topological taxonomy, basic correlations

SCIENTIFIC ORGANIZATION

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ABSTRACT

General taxonomy for chained coordination polymers was created. Each structure was characterized by 2-periodic rod and rod-packing nets. First one describes a connectivity of each chain, the second one – geometrical packing. For more detailed classification we used the following descriptors: composition of chain, type and coordination properties of ligands and central atoms. The values of calculated descriptors were stored in the “Knowledge database” of coordination polymers.

KEYWORDS

Coordination polymers (CPs), chain, 1-periodic, 1-dimensional (1D), taxonomy, classification, rod packings, underlying net, topology, geometrical and topological descriptors, secondary building unit (SBU).

ACKNOWLEDGEMENTS

Authors thank Russian government (grant No. 14.B25.31.0005) for support.

SUMMARY

The one-periodic coordination polymers (CPs) attract a great attention due to their electron and ionic conductivity, adsorption, catalytic and magnetic properties [1]. The exponential growth of the 1D complexes number indicates the persistent interest to them. However, accumulated crystallographic information is poorly used for finding general principals of their structural organization, developing the concept of their formation and searching correlations with properties. It requires further study and systematization in accordance to known crystallochemical descriptors and new ones. For example, the interesting parameters are the packing motif of rods and geometrical-topological characteristics of their external and internal cavities. The main goal of our work was to create the general geometrical-topological taxonomy for one-periodic coordination polymers.

Using ToposPro [2] we extracted from CSD (version 5.36) and analyzed crystal data for 26208 one-periodic coordination polymers. In result, we found the topological correlations driving structural organization of 1D coordination polymers. For example, we enumerated all observed rod-packings and probable relations between the local characteristics of inter-rod interactions and the type of packing. Interestingly, the same types of rod packings are observed for MOFs [3]. Further, we classified the 1D CP according to their composition and topological types, as well as coordination properties of central atoms and ligands. The values of calculated descriptors were stored in the “Knowledge database” of coordination polymers and can be used in “Expert system” for prediction of new compounds with specified properties and composition [4]. The results will be used for prediction of new structures and their properties.

Authors thank Russian government (grant No. 14.B25.31.0005) for support.

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Multifunctional nanostructured carriers with controllable sensitivity to ultrasound for theranostics

SCIENTIFIC ORGANIZATION

Saratov State University

ABSTRACT

New type of drug delivery carriers that will combine some functions as in vivo navigation and visualization, sensing of important biological marker, remote release of bioactive substances by external influences has a good perspective for applications in biomedicine. It was demonstrated that by control of nano- and microarchitecture of prepared surface, core-shell structures and capsule and also by variation of surface hydrophobicity, volume fraction and chemical composition of polyelectrolyte and inorganic nanoparticles can be change a sensitivity of carriers to ultrasound.

KEYWORDS

Nanostructured carrires,drug delivery, sensitivity to ultrasound, remote release, theranostics.

ACKNOWLEDGEMENTS

The reported study was supported by Government of the Russian Federation (grant №14.Z50.31.0004 to support scientific research projects implemented under the supervision of leading scientists at Russian institutions and Russian institutions of higher education).

SUMMARY

Theranostics defines the unique technologies that combine both medical diagnostics and therapeutics. Magnetite nanoparticles are a nice example of theranostic objects that can be used as MRI contrast agents and carrier for hypothermia induced by alternating magnetic fields. Other directions of theranostics are connected with nanostructured carrier applications. The Layer by Layer assembly technique is a power tool for creation of nanostructured multifunctional carriers combined sensing and drug delivery [1]. It was demonstrated that the sensitivity of capsule and core-shell to external influences as laser irradiation [2], magnetic field [2], ultrasound treatment [3] can be changed by variation of volume fraction and chemical composition of inorganic nanoparticles in the polyelectrolyte/nanoparticle shell. Same approach is applied for theranostic carrier visualization by MRI [4] and photoacoustic method [5] using magnetite and gold nanoparticles as contrast agents, respectively. Recently, it was shown the possibility to create a nanostructured SERS platform based on core-shell and capsules decorated by gold nanoparticles for studies of the chemical composition inside living cells [6]. This new type of object can be named satellite that can be used for studies of the microworld inside living organisms and their treatment on the cellular level and also for monitoring of implant/tissue interfaces [6].

The most important aspect is obtaining sensitivity of objects to external influences including ultrasound for remote release of bioactive substances realization. It was demonstrated that by control of nano- and microarchitecture of prepared surface, core-shell structures and capsule and also by variation of surface hydrophobicity, volume fraction and chemical composition of polyelectrolyte and inorganic nanoparticles can be change a sensitivity of prepared objects to ultrasound.

Obtained results are very important for creation of new generation of drug delivery systems including drug depot, combined much functionality as navigation and visualization, in vivo monitoring of biochemical process, remote activated release of bioactive substances in vivo by ultrasound.

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New optically active nanomaterials

SCIENTIFIC ORGANIZATION

Trinity College Dublin

ABSTRACT

The main goal of our research is to develop new types of technologically important optically active nanomaterials, study their properties and explore their applications. The utilisation of chiral stabilisers allowed the preparation of new water soluble white emitting quantum dots, rods, nano-tetrapods and nano-sheets, which demonstrated circular dichroism in the band-edge region of the spectrum. It is expected that optically active nanomaterials will find a range of potential uses in the chemistry, nanobiotechnology, photonics and optical chiral chemo- and bio-sensing.

KEYWORDS

Quantum dots, chirality, optical activity, nanotechnology.

ACKNOWLEDGEMENTS

The authors acknowledge financial support from EU FP7 programme (Future Nanoneeds grant, #604602), the Science Foundation of Ireland (Grant SFI 12/IA/1300), the Government of the Russian Federation (Grant 074-U01), and the Ministry of Education and Science of the Russian Federation (Grant No. 14.B25.31.0002).

SUMMARY

The area of optically active metal nanoparticles has received a great deal of attention due to the range of potential applications offered by these materials in chiral sensing, catalysis and as metamaterials in advanced optical devices . The use of stereospecific chiral stabilising molecules has also opened another avenue of interest in the area of optically active quantum dot (QD) research. Initially, optically active CdS QDs have been prepared by us using microwave induced heating with the racemic (Rac), D- and L-enantiomeric forms of penicillamine as stabilisers. Circular dichroism (CD) studies of these QDs have shown that D- and L-penicillamine stabilised particles produced mirror image CD spectra, while the particles prepared with a Rac mixture showed only a very weak signal It was also found that all three types of CdS particles (D-, L-, and Rac penicillamine) show very broad emission bands between 400 and 700 nm due to defects or trap states on the surfaces of the nanocrystals. We have also reported chiral CdSe QDs and chiral CdS nanotetrapods. All of these chiral nanostructures also showed a very broad distribution of photoluminescence which originates from emissive defect states and characteristic CD responses within the band-edge region of the spectrum. More recently we have reported intrinsic chirality of CdSe/ZnS QDs, which is caused by the presence of naturally occurring chiral defects (e.g. dislocations) and not by the presence of chiral ligands . Using theoretical modeling we have also demonstrated that optical activity can be inherent to many semiconductor nanostructures (e.g. nanowires and nanorods), as it is induced by chiral screw dislocations naturally developing

during their growth. Finally, using a combination of exfoliation and phase transfer techniques, we have developed a range of optically active two dimensional (2D) nanostructures such as MoS_2 and WS_2. These nanostructures have demonstrated strong unique CD responses and very interesting structural morphology. It is expected that optically active nanomaterials will find a range of potential uses in the chemistry, nanobiotechnology, photonics and optical chiral chemo- and bio-sensing. In addition, optically active quantum nanostructures can find applications as circular polarized light emitters and new metamaterials.

Ivanov Alexey
Junior Scientist

Novel materials with mixed ionic-electronic conductivity for solid oxide fuel cell technologies

SCIENTIFIC ORGANIZATION

Institute of Solid State Physics

ABSTRACT

One of the important challenges in developments commercially feasible intermediate temperature solid oxide fuel cells (SOFCs) relates to electrode materials and systems proving with sufficient stability and high electrochemical activity at operation conditions. The present work is centered on the studies of stability, oxygen nonstoichiometry, conductivity and ion transference numbers of Ce1-x-yLaxPryO2-δ, where the partial substitution of Pr4+/3+ cations for cerium makes it possible to improve p-type electronic transport under the SOFC cathodic conditions.

KEYWORDS

SOFC, protective interlayer, conductivity, oxygen permeability, Seebeck coefficient, cation interdiffusion, oxygen nonstoichiometry.

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation (project 14.B25.31.0018).

SUMMARY

Single-phase powders of $Ce_{1-x-y}La_xPr_yO_{2-\delta}$ (x=0.29-0.40, y=0-0.20) with submicron particle size were synthesized by the glycine-nitrate technique. Following firing at 1073 K and ball-milling in ethanol, final annealing of the powders was carried out at 1223 K in air for 4 h. Gas-tight ceramics (relative density >92%) were uniaxially compacted at ~100 MPa and then sintered at 1723 K for 20 h. The materials were characterized by XRD, SEM, and measurements of the total conductivity, Seebeck coefficient, oxygen nonstoichiometry, thermal and chemical expansions, transference numbers and steady-state oxygen permeation as function of the oxygen partial pressure and temperature. In order to evaluate chemical compatibility with solid oxide electrolytes, powder mixtures of $(Ce,La,Pr)O_{2-\delta}$ and $La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ or 8 mol.% yttria-stabilized zirconia (1:1 weight ratio) were fired at 1473-1623 K for 50-70 h. Model electrochemical cells with $La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ solid electrolyte, $(Ce,La,Pr)O_{2-\delta}$ interlayers and various perovskite electrodes were fabricated using screen-printing and annealing at 1373-1473 K, and characterized by impedance spectroscopy.

The results showed that, as expected, Pr doping leads to a higher p-type electronic conductivity under oxidizing conditions, whilst the ionic conductivity variations are determined by the [Ce]/([La]+[Pr]) ratio. The steady-state oxygen permeability is limited by the hole transport and, hence, correlates with praseodymium concentration. The variations of n-type electronic conductivity under reducing conditions, when most Pr cations are trivalent, can be described by classical defect models similar to those for ceria. XRD and SEM analyses of the reacted mixtures demonstrated that chemical interaction between $(Ce,La,Pr)O_{2-\delta}$, $La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ and zirconia cannot be neglected, at least at temperatures above 1500-1550 K. The electrochemical cell fabrication temperature should therefore be minimized down to 1373-1473 K. Nevertheless, these temperatures are sufficient to produce porous interlayers with high mechanical strength and sufficient adhesion to the solid electrolyte membranes.

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Doctor of chemical Sciences

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Nanomedicine & drug delivery, pharmacoengineering

SCIENTIFIC ORGANIZATION

University of North Carolina at Chapel Hill /M.V. Lomonosov Moscow State University

ABSTRACT

"Nanozyme" technology incorporates proteins into nanosized core-shell polyion complex particles that preserve even very fragile proteins in biological milieu, decrease their clearance and allow their site-specific delivery across cellular barriers. Examples include nanozymes based on antioxidant enzymes , scavengers of organophosphorous toxins and neurotrophins for treatments of obesity, stroke, Parkinson's disease, RETT syndrome, organophosphorous toxins poisoning, and some others.

KEYWORDS

Nanomedicine, nanozyme, drug delivery.

ACKNOWLEDGEMENTS

The research has been supported by the US National Institutes of Health, Rett.org and the Ministry of Education and Technology of Russian Federation.

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PhD

Leading Researcher

Development of novel palladium-containing catalysts on the basis of nanostructured polymers in hydrogenation and cross-coupling reactions for production of biologically active compounds

SCIENTIFIC ORGANIZATION

Tver State University

ABSTRACT

The increasing needs for production of the chemical and pharmaceutical and food industry demand development of new methods of obtaining of biologically active compounds. Proposed approach is based on the use of porous matrix of hypercrosslinked polystyrene (HPS) as a support for synthesis and stabilization of palladium nanoparticles. Thus the optimal procedure for HPS pretreatment was developed. This procedure was clarified from the point of view of support leaching, and it was found that no leaching of HPS takes place.

KEYWORDS

Kinetics, adsorption-desorption equilibrium, catalytic hydrogenation, Suzuki cross-coupling, palladium nanoparticles, palladium complexes, hypercrosslinked polystyrene.

ACKNOWLEDGEMENTS

The study was performed by the grant of Russian Science Foundation (project No. 15-19-20023).

SUMMARY

The increasing needs for production of the chemical and pharmaceutical and food industry demand development of new methods of obtaining of biologically active compounds. Reactions of selective catalytic hydrogenation (and selective hydrogenation of alkynols, in particular) are the basis of a number of existing syntheses. For example, product of 2-methyl-3-butyne-2-ol (MBY) hydrogenation (2-methyl-3-butene-2-ol (MBE)) can be further used to produce dehydrolinalool (DHL), selective hydrogenation of which results in formation of linalool (LN) – one of the most widely used terpene alcohols. One of the routes to LN production is acetylenic process. High space-time yields at reasonable selectivities (i.e., avoiding overhydrogenation) are required for the design of an efficient and economic process of obtaining of ethylene alcohols (e.g., MBE, LN, isophytol (IP)). About a half of worldwide LN

production is reckoned to be made through chemical synthesis while the rest is produced from natural plant terpenes. Most of produced LN (more than 95%) is used as a fragrance or flavouring agent. Moreover, LN can be regarded as a basic material for a very large range of other terpenoids. It can be converted to terpineol, geraniol and citral, and used in the preparation of citronellol, the ionones, farnesol and sesquiterpenes. Synthesis of fat-soluble vitamins (E and A) usually not involve LN, but its precursor DHL. The industrial method of alkynol hydrogenation is based on the use of Lindlar catalyst (Pd/CaCO3 modified with lead acetate and quinoline), which provides selectivity about 95% at 100% of conversion. Modification of Pd surface with quinoline was proposed to influence the polarization of the Pd-H bond due to the possible electron donation. Besides, it can compete with alkyne for adsorption and prevent polymerization and isomerisation processes. However, the use of these modifiers leads to pollution of target product that is inadmissible in pharmaceutical industry. In spite of numerous data on the MBY hydrogenation, it is still a challenge to achieve high selectivity in hydrogenation of terminal alkynes. On the other hand, the analysis of all possible factors influencing the alkene selectivity (the ability to form a certain hydride phase, the preferential alkyne adsorption, definition of small ensembles in order to reduce oligomerization), the size of Pd nanoparticles seems to be the key factor of a triple bond hydrogenation. At the same time, another challenge is to provide high stability of catalytically active Pd nanoparticles, as carbonization of palladium surface as well as sintering and leaching of nanoparticles often cause the loss of catalytic activity and selectivity at multiple reuses. It is noteworthy that during the development of new effective catalytic systems the use of nanostructured polymers as supports causes increasing interest. Polymers as supports are able to provide control over the particle size and their monodispersion that is the main problem of synthesis catalytically active metal nanoparticles. Besides, polymers have variety of properties (existence of functional groups, molecular weight, crosslinking degree, hydrophilicity or hydrophobicity, etc.), varying which it is possible to influence effectively processes of nanoparticle formation. Cross-coupling reaction is of the second importance in fine organic synthesis. Suzuki cross-coupling between aryl halides and arylboronic acids is one of the most widespread and effective methods of synthesis of biaryl, which are important semi-products in synthesis of pharmaceuticals, ligands and polymers. There are more than three hundred various commercial compounds which can react Suzuki. Suzuki reaction gives possibility to produce compounds possessing strong pharmacological activity which are rarely found in nature. In the case of reaction of Suzuki cross-coupling, which is also catalyzed by Pd, at present the most perspective catalysts are systems on the basis of Pd nanoparticles or complexes stabilized by polymers. However, in spite of success achieved in some cases, common disadvantage of heterogeneous, heterogenized and quasi-homogeneous catalysts of Suzuki reaction is loss of catalytic activity as a result of palladium leaching. The molecular forms of palladium formed in situ were considered as the most active ones, and though the complete prevention of Pd leaching is mechanistically impossible, it should be minimized. Besides, the disadvantage of many catalytic systems including polymer-stabilized Pd nanoparticles is the necessity of addition of phase transfer agent in order to achieve high activity in Suzuki reaction proceeding in aqueous medium. Proposed approach is based on the use of porous matrix of hypercrosslinked polystyrene (HPS) as a support for synthesis and stabilization of palladium nanoparticles. Among the organic porous supports, HPS, which is obtained by chemical incorporation of methylene groups between the neighboring phenyl rings in the polystyrene homopolymer solution in dichloroethylene or in a gel-like poly(styrene-p-divinylbenzyl) copolymer received increased attention. Due to its high crosslinking degree, which can be higher than 100%, HPS consists of rigid cavities (pores), the size of which can be varied depending on the reaction conditions. The unique property of HPS is the ability to swell in different solvents, which favors inclusion of various organometallic compounds in the HPS matrix. The existence of the pores of a standard size and shape allows controlling the metal particle growth. HPS-based catalysts allow control of the nanoparticle formation due to a “cage” effect (by limiting the nanoparticle size with the pore size) along with controlling the precursors and reduction conditions. It is noteworthy that HPS is commercially available. Another advantages of HPS are high thermal (up to 300°C), chemical and functional stability. It is noteworthy that HPS matrix also provides excellent stability of the catalytic systems due to the preventing of metal species dissolving and leaching. The above mentioned advantages of HPS make possible the multiple repeated use and regeneration of the developed catalysts. In general, the advantages of developed HPS-based catalytic systems in comparison with existing industrial catalysts include: (i) large specific surface area (usually near 1000-1500 m2/g); (ii) possibility to work in virtually any solvent; (iii) high catalyst

activity at lower metal loading due to formation of well-defined nanoparticles vs. their aggregation in conventional catalysts; (iv) higher stability and lifetime due to the minimization of metal loss; (v) high selectivity without necessity to use catalytic poisons and metal-modifiers; (vi) high activity without necessity to use phase transfer agents; (vii) prevention of nanoparticle aggregation during the reaction. Thus for the development of HPS-based catalytic systems, we used various HPS (non-functionalized and HPS bearing amino-groups). Besides, the nature of the metal precursor was varied to design nanoparticulate catalysts containing monodisperse nanoparticles. Catalysts based on HPS were synthesized by wet impregnation method followed by reduction of metal compounds. It is noteworthy that the impregnation method is simple in implementation, does not require complex laboratory equipment, does not need the use of the inert atmosphere (due to the high stability of HPS (chemical and thermal), and also palladium precursors). During the synthesis of polymer-containing HPS-based catalysts, the choice of a precursor is important. Depending on the precursor nature, it is possible to obtain catalysts with different distribution of active metal in the polymeric matrix that leads to formation of nanoparticles of different diameters. It is due to the hydrophobic nature of HPS matrix, which often does not allow hydrophilic metal precursor (acid or salt) to penetrate deeply into the polymeric network. During the catalyst synthesis, various precursors were used (PdCl2, Pd(CH3COO)2, (CH3CN)2PdCl2, (PhCN)2PdCl2, ((Sty)(CH3CN)PdCl2) and (Sty)2PdCl2) to control nanoparticle size and size distribution. Besides, metal loading and reduction method were varied (liquid-phase or gas-phase reduction). Unreduced catalysts, as a rule, show higher activity in cross-coupling reactions. However the development of effective catalyst on the basis of preliminarily created nanoparticles is possible. Therefore the question of a choice of the reduction method of metal catalyst is also important. In case of catalytic hydrogenation, liquid-phase reduction, which allows varying the rate of nanoparticle nucleation and, therefore, their diameter, is preferable. However, in view of the fact that the HPS possesses high thermal stability, gas-phase reduction in hydrogen flow, which is the most preferable in case of Suzuki reaction, is also possible. Thus in the case of the use of gas-phase reduction method in hydrogen flow, it is necessary to know the limits of temperature stability of the chosen polymer. In order to find the thermal stability of HPS polymeric matrix, thermogravimetric analysis of the polymeric matrix, which was pretreated and crushed up to sizes of granules less than 60 microns, was carried out. It was revealed that HPS is stable up to 300°C in argon medium; however, at higher temperatures the destruction takes place with the loss of about 60% of weight. Thus, the HPS-based catalysts can be reduced in hydrogen flow at a temperature 300°C without the risk of destruction of polymer structure. It was also found that for successful catalyst synthesis, initial HPS should be pretreated, to avoid the presence of inorganic impurities (Fe3+, Cl-) and to achieve low humidity (less than 2%). Thus the optimal procedure for HPS pretreatment was developed. This procedure was clarified from the point of view of support leaching, and it was found that no leaching of HPS takes place. To exclude internal diffusion limitations and to provide higher surface area HPS should be powdered before the use as support. As a result it was found that the use of HPS having granules size smaller than 60 μm is optimal.

Labutin Timur

Ph. D.

Senior researcher

The improvement of laser-induced breakdown spectroscopy

SCIENTIFIC ORGANIZATION

Lomonosov Mosocow State University

ABSTRACT

The achievements in the determination of trace amounts of components in environmental samples (soils, ores, natural waters, etc.) and construction materials by application of enhanced variant of laser-induced breakdown spectrometry are considered. Our results are critically compared with the state-of-the art in the field.

KEYWORDS

Laser induced breakdown spectrosocopy, analytical spectrosocpy, direct analysis, laser ablation.

SUMMARY

High-power pulsed laser radiation is used both for sample evaporation and excitation in laser-induced breakdown spectroscopy (LIBS), and the spectra of laser-induced plasma are used for quantitative and qualitative analysis. Fully optical excitation and detection provide the possibilities of local and remote analysis of light and heavy elements. The key advantages of the method that account for its high efficiency are demonstrated, in particular, a small amount of analyzed material, the absence of sample preparation, the possibility of local and remote analysis of either one or several elements. However, similarly to other direct methods matrix effects, sensitivity, and reproducibility are the main limitation the LIBS practical application. This study was carried out on improving the LIBS technique to overcome these problems, especially for geological samples and constructional materials.

We used a variety of techniques for increasing LIBS sensitivity including the use of different laser harmonics, double pulses, and a special mode of camera operation. We also suggested several approaches of improving the reproducibility of the analytical LIBS signal. We focused on algorithm of “internal” standard selection to correct pulse to pulse fluctuations, matrix effect, changing the laser parameters and environmental conditions. Application of these enhancements has led to a significant improvement in the detection limits for the number of elements, which are import markers in natural materials. The achieved limits of detection for most elements in geochemical samples are critically evaluated. We have shown that the possibilities of LIBS for quantitative determination of metals (Ni, Cr, Mn, Al, V, Ti) and nonmetal (Si, C) in high and low alloy steels are met the requirements of existing regulatory documents.

Linkov Pavel

Junior researcher

CdSe/ZnS/CdS/ZnS QDs with advanced two-photon properties for tumor diagnosis and treatment

SCIENTIFIC ORGANIZATION

National Research Nuclear University MEPhI

ABSTRACT

We propose a universal procedure for the synthesis of highly luminescent different size CdSe/ZnS/CdS/ZnS core/shell quantum dots, whose structure is based on charge carrier confinement engineering and which have highly uniform epitaxial shells and photoluminescence quantum yields as high as 100%. The obtained data of the two-photon properties demonstrate, that the large two-photon excitation action cross section makes synthesized core/multishell QDs a promising photoluminescent material for engineering of bright nanoprobes for multiphoton microscopy.

KEYWORDS

Quantum dots, semiconductor nanocrystals, two-photon labels, two-photon microscopy.

ACKNOWLEDGEMENTS

This study was supported by the Ministry of Education and Science of the Russian Federation, State Contract no. 4.624.2014/K.

SUMMARY

The current strategy for development of advanced methods of tumor treatment focuses on targeted drug delivery to tumor cells. Linking an imaging (fluorescence) agent to a biomarker recognizing molecule conjugated with the pharmacological agent ensures real-time tracking of the delivery of the active substance. Quantum dots (QDs) are semiconductor photoluminescent nanocrystals[1] with unique fluorescent characteristics: size-tunable light emission, a high signal brightness, and values of two-photon absorption cross section orders of magnitude higher than those of organic molecules. Thus, water-soluble QDs can be used as efficient biomedical fluorescent labels operating in the two-photon excitation mode, with fluorescence in the visible spectral range excited by irradiation of the QDs in the biological tissue transparency window[2].

Here, we have used an advanced procedure of the synthesis of highly luminescent QDs based on charge carrier confinement engineering developed earlier to synthesize core–multishell QDs (CdSe/ZnS/CdS/ZnS) with different sizes[3]. The QD cores were obtained by the hot-injection method1 using cadmium n-hexadecylphosphonate and selenium tri-n-octylphosphine complex as precursors, tri-n-octylamine as a stabilizing additive, and 1-octadecene as a solvent[3]. Then, purified CdSe cores were coated with a ZnS/CdS/ZnS shell three monolayers in thickness with the use of the SILAR (Successive Ionic Layer Adsorption and Reaction) approach. This shell structure provides a high potential barrier for effective protection of excited charge carriers from the environment. As a result, we obtained series of highly luminescent CdSe/ZnS/CdS/ZnS QDs with emission wavelength maxima at 540, 575, and 610 nm and PL quantum yields of 90, 97, and 80%, respectively.

We also studied the two-photon properties of three series of the synthesized QDs in chloroform[4]. The two-photon excitation action cross-sections of QD-540, QD-570, and QD-610 were found to be 11,000, 16,000, and 13,000 GM, respectively (1 GM = 10^{50} cm^4 s/photon)[5]. These values are comparable with those of the best samples of CdSe/ZnS QDs and are three orders of magnitude higher than those of conventional organic fluorophores.

The large two-photon excitation action cross sections make the synthesized nanocrystals excellent photoluminescent materials for engineering of bright nanoprobes for multiphoton microscopy. Thus, the core/multishell QDs with a bright PL in the one- and two-photon modes can be used for engineering of small-sized fluorescence labels for tumor diagnosis and treatment systems capable of penetrating into live cells.

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SCIENTIFIC ORGANIZATION

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ABSTRACT

Heterogeneous catalysis has a wide range of applications in a large number of processes in oil refining, petro- and chemical industry. The presentation will focus on catalyst shaping aiming at production of catalyst granules with specified physical and chemical properties, such as specific surface area, optimal pore size distribution, mechanical strength of grains and active phase distribution across a granule.

KEYWORDS

Catalysis.

SUMMARY

- advanced fuels;
- process intensification;
- catalytic processes in oil and petrochemical industry.

Nazarov Denis
Graduate student

Synthesis of biocompatible coatings of high value of micro- and nanoroughness based on titanoxide structures on the surface of nanostructured titanium

SCIENTIFIC ORGANIZATION

Saint-Petersburg State University, Institute of chemistry

ABSTRACT

The chemical etching of coarse and ultrafine titanium has been studied in detail in this work. Significant effect of the nature and concentration of the etchant, the time of the process on the micro and nanoroughness and composition of the titanium surface was observed. Coatings with the required topography and composition for use as bone and dental implants were produced by chemical etching and deposition of layers containing titanoxide, organotitanium, and phosphate chemical groups.

KEYWORDS

Surface modification, nanostructured titanium,etching media, ALD, biocompatibility, bioactivity.

ACKNOWLEDGEMENTS

The study was fi nancially supported by megagrants of the Ministry of Education and Science of the Russian Federation (Contract no. 14.B25.31.0017).

SUMMARY

The coarse grain metallic materials are traditionally used in dental and orthopedic implants. However, they already reached their limit of the constructive strength, plasticity and other mechanical properties. In this regard, the great interest exists in recent years to nanostructured materials (NM). Especially interesting are the metals obtained by means of the intensive plastic deformation (IPD). Numerous works [1-3] demonstrate that the nanostructuring by means of IPD can provide the meaningful improvement of the mechanical properties of the pure titanium (that is the most suitable material for the medical implants.

However, the mechanical properties are not the only characteristic for the suitability of implant materials. Much more important characteristics are their bioinertness,

biocompatibility, and bioactivity. Titanium bioinertness and biocompatibility are acceptable for the implantology due to the presence of natural oxide layer. At the same time, very important task is the improvement of titanium bioactivity. Bioactivity can be improved either by the surface modification and biocovering or by the variation of the surface relief [4, 5]. The developed bioactive relief is usually formed by means of mechanical treatment, electrochemical or chemical etching. To date a lot of research materials in this area are accumulated. However, there are only few works on the modification of highly promising nanostructured titanium. Nevertheless, physicochemical properties and the etching mode for nanostructured titanium are significantly different from ones for coarse grain titanium.

In this regard, first part of work is dedicated to the study of the dependence between titanium grain size, relief and composition of the surface while the treatment with different etchants in the range of etching times (from 5 min to 24 h). Initial coarse grain titanium Grade 4 with the average grain size of 25 nm and ultrafine titanium, obtained by IPD with the average grain size of 100 nm were disks of 12 and 6 mm in diameter and with 2-3 mm thickness, respectively. These disks were polished until roughness level of 3-5 nm. As the etching media, we used acidic (H_2SO_4/H_2O_2) and alkaline (NH_4OH/H_2O_2) Piranha solutions.

It is shown by means of SEM and AFM that for the samples of etched ultrafine and coarse grain titanium, the etching medium nature as well as time of exposure influence significantly on the titanium surface morphology. In the case of acidic Piranha solution, the spongy structure is formed. If the etching time is increased to 24 h, this structure is destroyed and the surface roughness is increased significantly (RMS increases from 5-7 nm to 42.1 nm). Coral-like structures are formed while using alkaline Piranha solution with exposure times up to 2 h. Further treatment converts these structures to netlike ones (with net size of 50 to 200 nm depending on $NH_4OH\backslash H_2O_2$ ratio.

It is worth to note that the surface of the samples after treatment in $NH_4OH\backslash H_2O_2$ for more than 2 h is characterized by the presence of “holes” with 1-2 μm in diameter and depth up to 10-20 μm. Besides, the data of X-Ray Photoelectron Spectroscopy demonstrate the peaks assigned to Ti^0 even after prolonged etching in ammonia solution. These peaks are not found for the samples treated in $H_2SO_4\backslash H_2O_2$. This fact shows that the surface oxidation by H_2O_2 is actively proceed in acidic medium and is almost inactive in ammonia medium. The comparison of ultrafine and coarse grain titanium demonstrates that the nanostructured titanium is etched more actively and more uniformly. At the same time, qualitative difference is not observed.

The second part of work describes the formation of biocompatible layers on etched nanostructured titanium by means of ALD. This method provides differently shaped thin layers on the substrates keeping the surface relief unchanged.

Titanium isopropoxide and water have been used as initial reagents to get titanorganic and titanoxide structures. Tert-butyl phosphate and water provided phosphate groups addition. The samples were synthesized at 250^0C and inert gas pressure of 20 mm Hg. 400 ALD cycles allowed to get 20-nm thick layers (data of spectral ellipsometry). The presence of titanorganic and phosphate groups has been confirmed by means of X-Ray Photoelectron Spectroscopy and X-Ray Fluorescent Analysis. The XPS data also demonstrate the absence of Ti0 characteristic peaks. This is the confirmation that the ultrafine titanium is covered by the film. According to SEM and AFM data, netlike and sponge-like structures are not preserved while layering, whereas the micron-sized “holes” remain unchanged after the film deposition. For all the samples the grains of 20-100 nm in diameter are indicative. It is worth to note that for ultrafine titanium etched in $NH_4OH\backslash H_2O_2$, the density of grain packing is much higher for 2 h etched sample compared to one etched for 15 min. For $H_2SO_4\backslash H_2O_2$ – treated samples, the exposure prolongation leads to appearance of grains.

In conclusion, the influence of various etching media was studied on the manner of etching of ultrafine and coarse grain titanium samples. It was shown experimentally that the biocompatible material can be created that combines well mechanical properties (ultrafine titanium), developed relief both on nano and micro levels, as well as the presence of titanium-oxygen layer with phosphate groups. This new material is able to provide high biocompatibility and bioactivity.

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ADDITIONAL INFORMATION

Co-authors: Zemtsova E.G., Soloxin A.Yu, Valiev R.Z. The study was fi nancially supported by megagrants of the Ministry of Education and Science of the Russian Federation (Contract no. 14.B25.31.0017).

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Genesis and structure of MoO3/ZrO2 solid acid catalysts of isobutene alkylation

SCIENTIFIC ORGANIZATION

Saint-Petersburg State Institute of Technology (technical university)

ABSTRACT

A series of solid acid catalysts composed of MoO_3/ZrO_2 were prepared by the methods of impregnation and mechanical mixture. By the methods of FTIR, X-ray diffraction, thermal gravimetric and differential thermal analysis, adsorption-desorption of nitrogen, pyridine adsorption and adsorption acid-base indicators showed a strong influence of the ratio MoO_3/ZrO_2, calcination temperature, type of MoO_3-precursor and preparation method on acidic surface characteristics, the pore structure and activity.

KEYWORDS

Zirconia, molybdenum oxide, alkylation, isobutane.

ACKNOWLEDGEMENTS

This work was executed at the Laboratory “Catalytic Technology” at St. Petersburg State Institute of Technology supported by the mega-grant of the Government of the Russian Federation. Also I express gratitude to the staff of laboratory “Catalytic Technology” to Fedorov S.P. in carrying out analyses of the porous structure and Matveeva A.N. in carrying out experiments on DTA-TGA.

SUMMARY

Introduction

Alkylation of butenes with alkanes results in high octane alkylates with a high octane number (above 94) used for both synthetic motor fuel production and for compounding of low octane number gasoline [1-3]. A promising direction in the development of alkylation processes is the transition from liquid-phase catalysts such as HF and H_2SO_4 to heterogeneous catalysis thus avoiding problems related to chemical corrosion of equipment, toxicity of waste acids and their disposal.

In the petrochemical synthesis widespread catalysts MoO_3 and WO_3, which are used in different processes: isomerization, cracking, hydrotreating. Alkylation is a complex process, which also includes the isomerization reaction. Therefore, it is logical to study ZrO_2-MoO_3 / WO_3 catalysts in the alkylation of isobutane with olefins.

For example, [4.5] shows the influence ratio and calcination temperature for ZrO_2-WO_3 catalyst at the value of the specific surface, ratio of ZrO_2 modifications, etc. In experiments on the alkylation of isobutane with olefins [5], such systems showed better activity and selectivity as compared to the sulfated zircinia (ZrO_2/SO_4) catalysts. MoO_3/ZrO_2 have not been studied in this process.

It should be noted that in the preparation of MoO_3/ZrO_2 catalysts are generally used methods of impregnation and coprecipitation. By mixing the initial components is given little attention.

In this work shows the influence the preparation method (impregnation or mixing), ratio of the initial components, type of MoO_3-precursors and calcination temperature on the physicochemical properties of the MoO_3/ZrO_2 catalysts.

Experimental part

Zirconium hydroxide ($Zr(OH)_4$) was prepared by precipitation from a 10% solution of zirconyl chloride solution at pH=9 by addition of 25% ammonium hydroxide solution. Then the precipitate was kept 1 hr under a mother liquor, then was filtered off on a vacuum filter. The resulting hydroxide is washed off by decantation from chlorine ions at pH=8 at the rate of 30 liters of water per 100g $ZrOCl_2$. The resulting solids were dried in air overnight at 373-383 K.

As MoO_3-precursors used: H_2MoO_4, $H_3PMo_{12}O_{40}$, $H_4SiMo_{12}O_{40}$ and $(NH_4)_6Mo_7O_{24}$.

Samples of the catalysts by mixing and impregnation were prepared. In the first series - mixing samples - changed Mo-precursor, content of MoO_3 (6,6 and 13,2% wt.) and calcination temperature (500, 600 and 700°C). The catalysts are represented by *Zr-XMo(Y)-T*, where X represents weight percentage of MoO_3, Y represents the type of MoO_3-precursor (H - H_2MoO_4, P - $H_3PMo_{12}O_{40}$, Si - $H_4SiMo_{12}O_{40}$), and T denotes calcination temperature (°C). In the second series of samples were compared preparation methods, treatment temperature and the MoO3-predecessor. The catalysts are represented by *Zr-600Mo(Y)-T*, where 600 represents wt. %MoO_3 at which MoO_3 covers zirconia with a monolayer, Y represents the type of MoO_3-precursor (NH_4 - $(NH_4)_6Mo_7O_{24}$, P - $H_3PMo_{12}O_{40}$), and T denotes calcination temperature (°C).

The specific surface areas (SSA) of the catalysts were measured by N_2 physisorption at liquid nitrogen temperature with a Quantachrome Autosorb 6 iSA and standard multipoint BET analysis methods.

X-ray diffraction (XRD) measurements of the catalyst powder were recorded with a Shimadzu XRD-7000 diffractometer equipped with Ni-filtered CuKα radiation (λ = 1.5418 Å). The volume percentage of the monoclinic phase (Vm) of the calcined samples was estimated with the formula proposed by Toraya et al. [6].

The nature of the acid sites (Brønsted and Lewis) of the catalyst samples was characterized by in situ FTIR spectroscopy (Shimadzu IrTracer-100) with chemisorbed pyridine. Also functional composition of the samples surface was investigated by adsorption of acid–base indicators with different pKa values ranging from -4.4 to 14.2, which were selectively adsorbed on the surface active sites with the corresponding pKa values a according to the method described in [7].

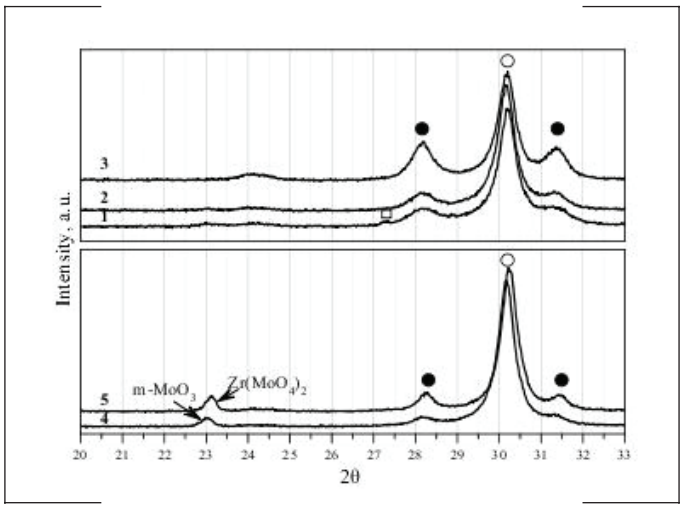
Differential Thermal and Thermo Gravimetric Analyis (DTA-TGA) was carried out on a Shimadzu DTH-60H using 0.02 g of sample, and heating in air from 25 to 800°C.

RESULTS

Figure 1 shows an example of XRD for Zr-XMo(Si)-T patterns with different MoO_3/ZrO_2 ratio. At 500°C and 6.6% wt. MoO_3 the phase composition of t-, m-ZrO_2 and o-MoO_3 is presented. Presumably, with increasing the calcination temperature there is a destruction of crystalline structure of MoO_3 and its further spreading of surface ZrO_2. With increasing wt.% MoO_3 to 13,2% and T=700°C there is formation of the new phase - $Zr(MoO_4)_2$ in the hexagonal modification, and also lack of the MoO_3 phase. Similar regularity is observed also when using the molybdic acid, however, but at 500°C phase of o-MoO_3 is formed, and at 600°C - m-MoO_3. When using 12-molybdophosphoric acid formation of $Zr(MoO_4)_2$ phase was not observed.

From XRD it is visible that calcination temperature increase results in an increase of the integral intensities m-ZrO_2. From Figure 2 shows the dependence Vm on wt.% MoO_3 in comparison with the pure ZrO_2 with different temperature calcination.

Fig.1. X-ray diffraction patterns of
1: Zr-6,6Mo(Si)-500;
2: Zr-6,6Mo(Si)-600;
3: Zr-6,6Mo(Si)-700;
4: Zr-13,2Mo(Si)-600;
5: Zr-13,2Mo(Si)-700
(• - m-ZrO2; ○ - t-ZrO2; □ – o-MoO3)



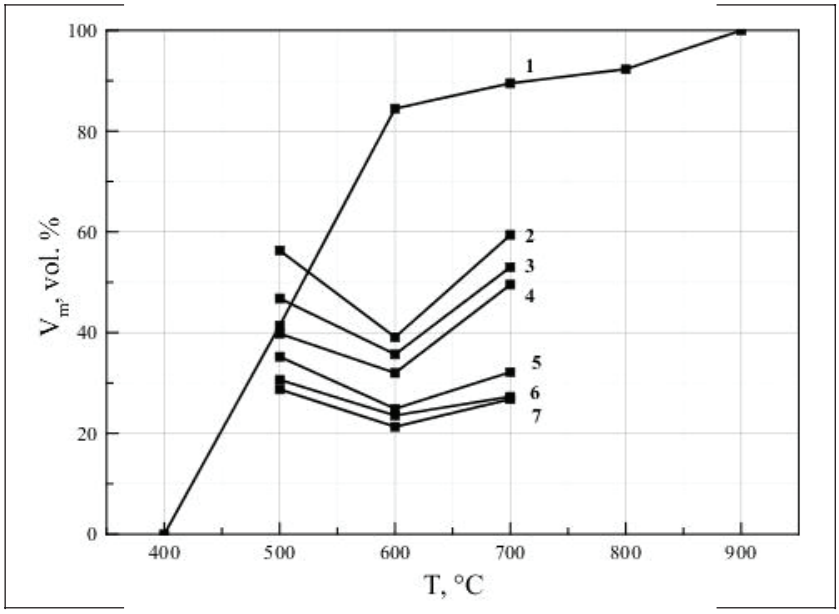


Fig.2. The dependence of the volume fraction (Vm) of m-ZrO_2 on the calcination temperature, the content MoO_3 and MoO_3-precursor 1: ZrO_2; 2: Zr-6.6Mo(H); 3: Zr-6.6Mo(Si); 4: Zr-6.6Mo(P); 5: Zr-13.2Mo(H); 6: Zr-13.2Mo(P); 7: Zr-13.2Mo(Si)

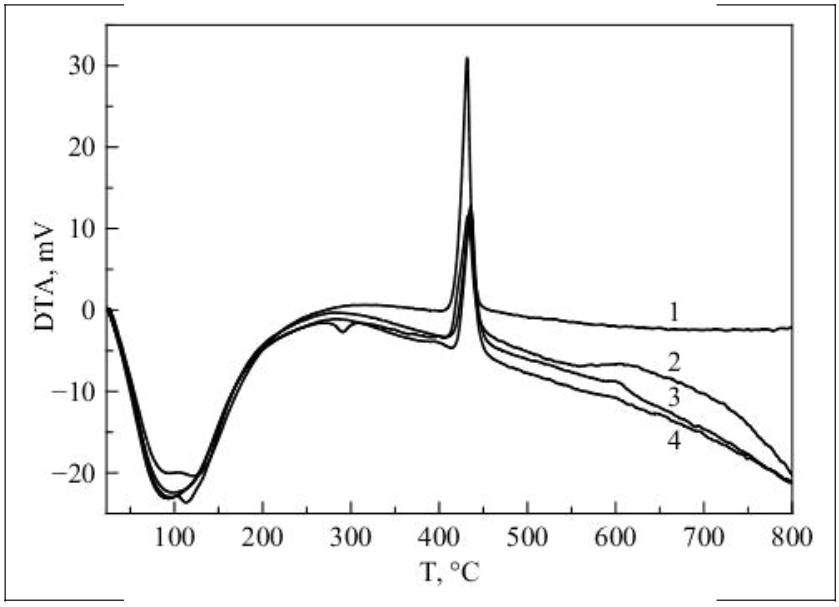


Fig.3. DTA-curves 1: $Zr(OH)_4$; 2: Zr-13,2Mo(P); 3: Zr-13,2Mo(H); 4: Zr-13,2Mo(Si)

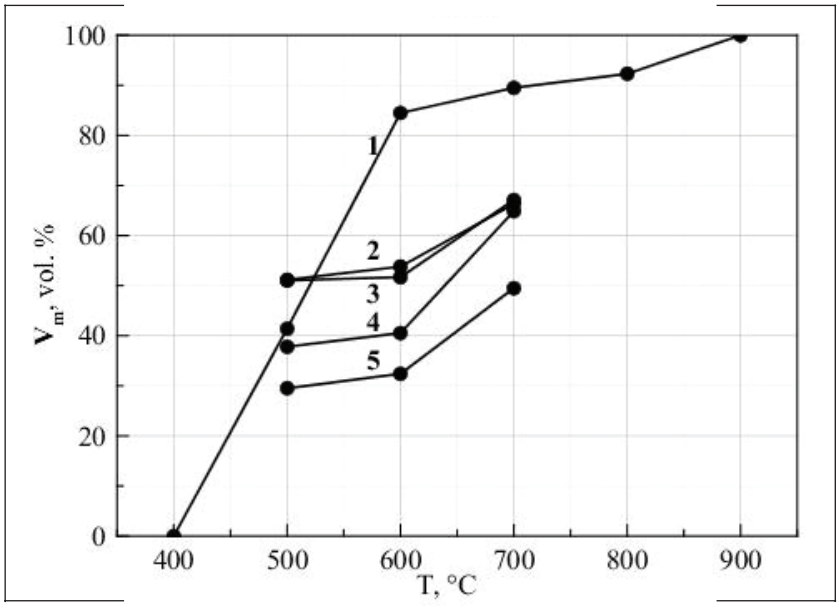


Fig.4. The dependence of the volume fraction (Vm) of m-ZrO_2 on the calcination temperature, preparation method and MoO_3-precursor 1: ZrO_2; 2: Zr-600Mo(P)$_{mix}$; 3: Zr-600Mo(NH_4)$_{mix}$; 4: Zr-600Mo(P)$_{imp}$; 5: Zr-600Mo(NH4)$_{imp}$

Minimum volume fraction falls to 600°C, which is associated with the destruction of the structure of MoO_3 phase, its distribution over the surface of the ZrO_2 and therefore t-ZrO_2 crystal growth delay. Increasing wt.% MoO_3 contributes to a greater slowdown in the growth of t-ZrO_2 crystals and their further transition to m-ZrO_2.

Figure 3 shows the results DTA for mixing samples Zr-13,2Mo(X). It can be seen that the exothermic peak (429°C), which corresponds to the crystallization of the amorphous ZrO_2 is not displaced. Consequently when mixing any of the solid acids does not prevent crystallization of the amorphous ZrO_2, which is explained by incomplete conversion of the starting Mo-compounds at 429°C.

In this sample series of content MoO_3=4,23% wt., which is calculated according to [8].

XRD shows that the phase composition of impregnation samples is presented by t- and m-ZrO_2, but also mixing additional m-MoO_3 phase using ammonium heptamolybdate. Figure 4 shows the results of calculations Vm, that indicate better stabilization of t-ZrO_2 when impregnation using ammonium heptamolybdate and somewhat poorer stabilization of t-ZrO_2 when impregnation using 12-molybdophosphoric acid.

DTA shows that by using the impregnation as the preparation method, there is a delay of amorphous oxide crystallization , i.e. crystallization temperature rises to 462°C (12-molybdophosphoric acid) and 470°C (ammonium heptamolybdate). Such influence preparation method has a positive effect on the value of the SSA (Fig. 5).

Result by adsorption-desorption of pyridine (Fig. 6) to mixture sample Zr-13,2Mo(P)-600 shown in Fig. 6 (shows FTIR of the residual adsorbed pyridine at different desorption temperatures T_{des}). From the results it follows that the sample surface is represented by different types of acid centers. Among the Lewis acid centers (LAC) is dominated by weak centers. Among the Brønsted acid centers (BAC) is dominated by strong centers. Presumably, LAC corresponds Zr^{4+} and BAC - Mo-OH and Zr-OH.

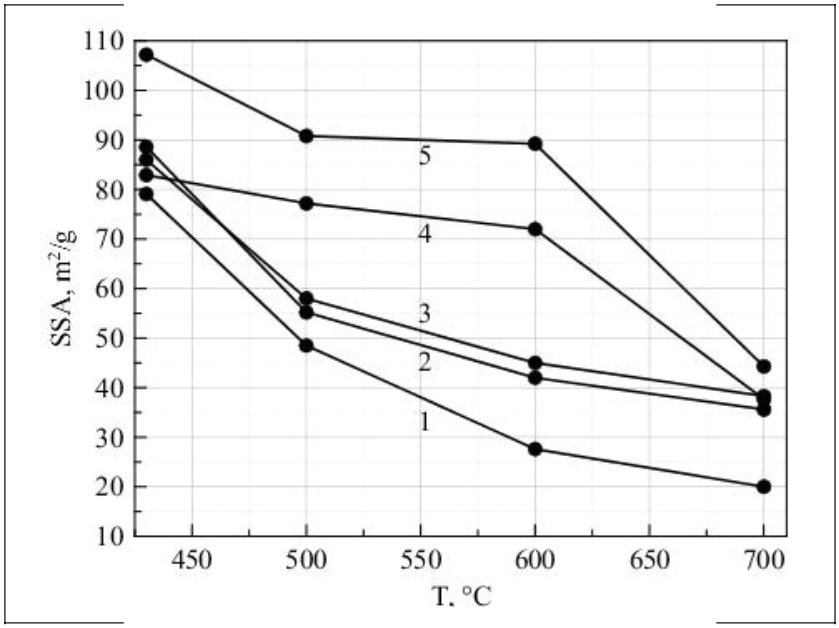


Fig.5. Depedence of SSA on calcination temperature 1: ZrO_2; 2: Zr-600Mo$(NH_4)_{mix}$; 3: Zr-600Mo$(P)_{mix}$; 4: Zr-600Mo$(NH_4)_{imp}$; 5: Zr-600Mo$(P)_{imp}$

Result by adsorption of acid–base indicators with different pKa to impregnate sample Zr-600Mo$(P)_{imp}$-600 shown in Fig. 7. Its surface is mainly represented by the LAC, but also contains minor amounts of other centers of acidic (BAC, strong and weak) and basic (BBC). A similar result for acid sites shows the adsorption-adsorption of pyridine.

CONCLUSIONS

The results obtained indicate a promising catalyst in the alkylation of isobutane with butenes. In the future we plan to explore the best samples in the alkylation of isobutane.

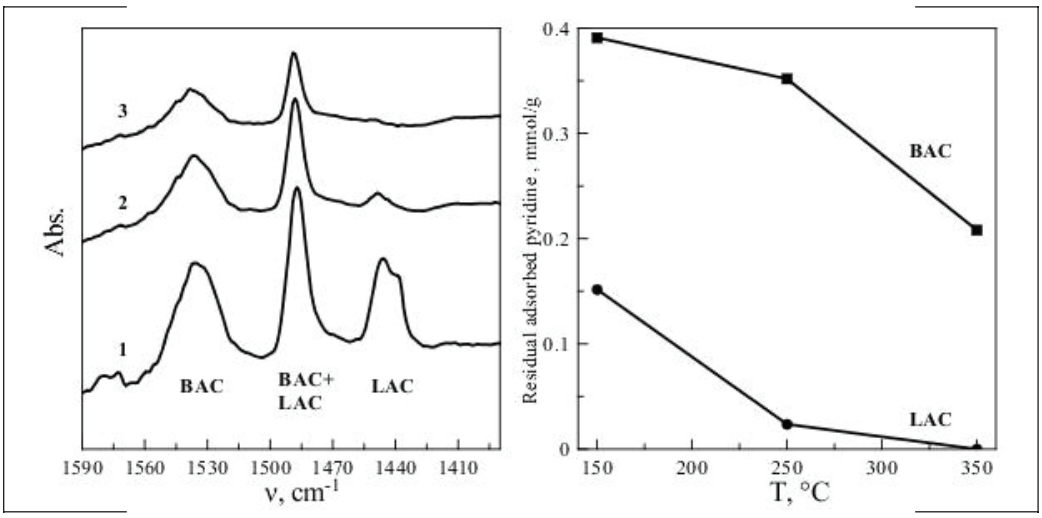


Fig.6. FTIR of the residual adsorbed pyridine on surface Zr-13,2Mo(P)-600; 1: T_{des}=150°C; 2: T_{des}=250°C; 3: T_{des}=350°C

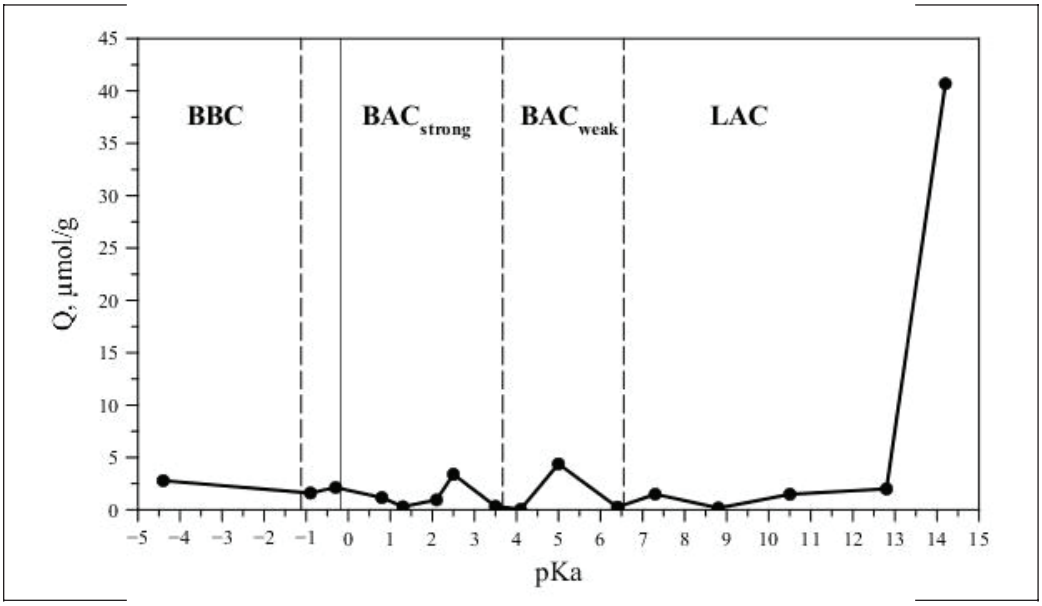


Fig.7. Distribution of adsorption centers on the surface of Zr-600Mo$(P)_{imp}$-600 catalysts

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Building Polymers For the Future: Toward Multifunctional Synthetic Macromolecules Inspired By Nature's Mechanisms of Action

SCIENTIFIC ORGANIZATION

National Center for Scientific Research - Centre National de la Recherche Scientifique

ABSTRACT

The past few decades have witnessed a vast improvement in the development of methodological tools available to synthetic chemists in their efforts to design organic (macro)molecules of different sizes, shapes, topologies, architectures and fonctionalities. This presentation will describe how these advances can be exploited in the field of synthetic macromolecules, focusing on efforts aimed at imparting biological attributes to large synthetic molecular systems and have them "compete" with biopolymers.

KEYWORDS

Polymer science, synthesis, biomimetics, macromolecules.

SUMMARY

- A comparison between biomacromolecules and currently available synthetic macromolecules (and their respective modes of action) can be a powerful way to design "advanced" polymers that hopefully combine the best of the two worlds.

- It requires the development of strategies to incorporate key elements (e.g., folding units, recognition sites) used by biomacromolecules into synthetic macromolecules.

- A description of a few examples will be provided to illustrate the above concept.

Proserpio Davide
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Periodic Structures and Crystal Chemistry

SCIENTIFIC ORGANIZATION

Università degli Studi di Milano

ABSTRACT

The history of the topological crystal chemistry approach will be outlined with the special contribution of the Samara Center for Theoretical material Science.

KEYWORDS

Crystallography, Metal-Organic Frameworks, topology of crystal structures, Structural Supramolecular Chemistry, Carbon Allotropes.

SUMMARY

In the rationalization process of complex structures it is very helpful the "topological approach" that consists in the simplification by rational principles of the complex structures to schematized reference *nets* [1]. A higher level of complexity comes from the entanglement of different periodic motifs whose rationalization and classification we have illustrated in the last years. The different branches of mathematics involved show the interdisciplinary approach of the Topological Crystal Chemistry developed in the Samara Center for Theoretical Material Science (SCTMS) www.sctms.ru

simplification and rationalization -> nets (graph theory) [1]

topological classification/analysis of nets [2,3]

- single/entangled/catenated/knotted (knot theory) [4,5]

- enumeration of nets and relation to carbon allotropes [6,7]

- tiling theory and zeolites [7]

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In situ click chemistry generation of candidate ligands for adenosine receptor A2A with a soluble adenosine binding protein template

KEYWORDS

Click chemistry.

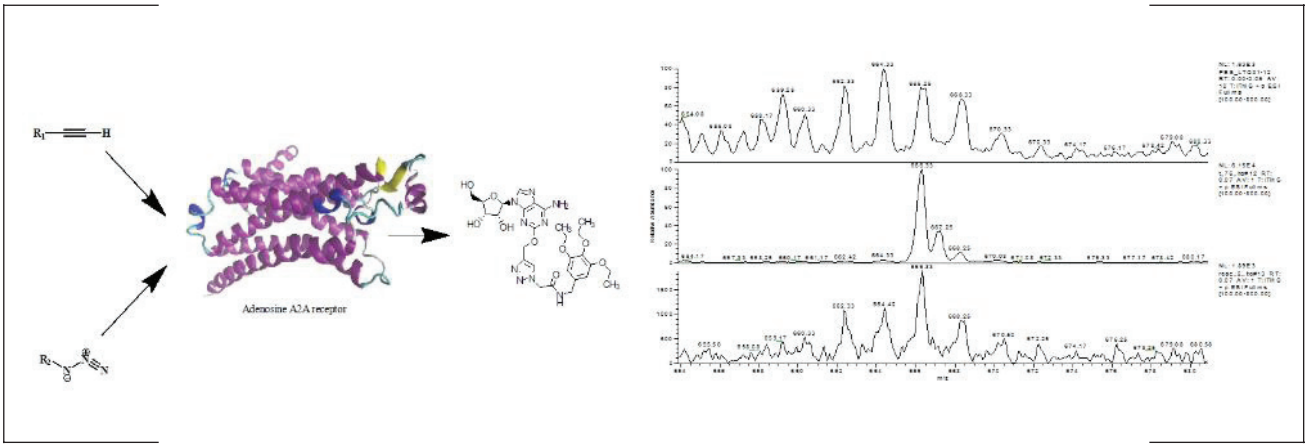
SUMMARY

Adenosine A2A receptor is a member of GPCR family which is responsible for regulating myocardial blood flow and also plays an important role in the regulation of glutamate and dopamine release, making it a potential therapeutic target for the treatment of conditions such as insomnia, pain, depression, drug addiction and Parkinson's disease.[1]

In this work, soluble adenosine A_{2A} receptor in 0.01M PBS with detergent was used as in situ template for generation of novel and potent ligands that selectively bind to this protein. The cycloaddition reaction between an anchor alkyne fragment and a library of azides that forms stable 1,2,3-triazoles was used to generate lead compounds. This bioorthogonal reaction is fully compatible with functional groups found in normal physiological environments.[2]

The process begins with selective binding of molecules containing an alkyne and azide groups to specific areas of the protein binding site. The two fragments that form a high-affinity ligand link together irreversibly within the confines of the template's binding pocket, thus forming of an energetically favorable complex with the protein. The extent of the triazole formation on A_{2A} template correlated with the affinity of the triazole product for the adenosine ligand binding site. We have modified adenosine via alkyne group and used it as an anchor reacting with over one hundred azides, dividing them into multiple sets. For the detection of triazoles, we used an ion trap mass spectrometry (amaZon SL, Bruker). As a result, eight preliminary hits were found.

In order to find the most affine ligands among these hits we performed one more experiment with A_{2A} receptor binded with ZM241385, a high affinity antagonist ligand selective for the receptor.[3] The intensity of found key triazole signal detected via ion trap mass spectrometry decreased at least two fold in comparison with the experiment without ZM241385.



The formation of the molecule was proved by comparison the results of high-resolution TOF ESMS+ spectra for triazole obtained on A2A template and the same molecule synthesized by Cu(II)-catalysed cycloaddition reaction.

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ADDITIONAL INFORMATION

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Self-cleaning coatings: Present and Future

SCIENTIFIC ORGANIZATION

Saint-Petersburg State University

ABSTRACT

Self-cleaning materials have considerable attention for both their unique properties and practical applications in energy and environmental areas. Factors influencing on photoinduced hydrophilic conversion are considered. Several strategies to improve the efficiency of photocatalytic and self-cleaning properties are demonstrated. Real time manipulation of hydrophilic/hydrophobic properties of semiconductor-based nano-coating surfaces caused by different factors is also an attractive topic due to its great practical importance.

KEYWORDS

Self-cleaning, photocatalysis, antibacterial, synthesis, wettability, photoinduced hydrophilicity.

ACKNOWLEDGEMENTS

The present study was performed within the Project “Establishment of the Laboratory “Photoactive Nanocomposite Materials” No. 14.Z50.31.0016 supported by a Mega-grant of the Government of the Russian Federation.

SUMMARY

Self-cleaning materials have considerable attention for both their unique properties and practical applications in energy and environmental areas. Since the effect of surface photoinduced superhydrophilicity was discovered in 1997 (Fig. 1) the TiO_2 based photocatalysts have gained considerable attention.

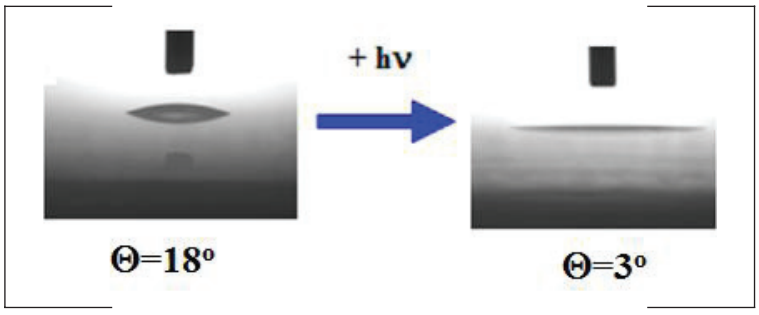

Figure 1. TiO_2 nano-coating: UV-induced superhydrophilic conversion.

Vigorous applied studies of the effect have resulted in the development of self-cleaning and anti-fogging glass, self-cleaning coating for exterior and interior surfaces for buildings, tunnels, and road shields and, so on. Despite to wide applications the understanding of mechanisms and reasons yielding the observation or non-observation of this effect on some metal oxide surfaces are still under discussion.

The present study explored the effects of several factors (namely, wetting, light intensity, spectral variation of the actinic light, heating, surface acidity) on the hydrophilic conversion of the surface of TiO_2 and ZnO nanocoatings. The experimental dependences of the efficiencies of photoinduced hydrophilic surface conversion on the intensity and wavelength of the actinic light clearly indicate the role of electronic photoexcitation in hydrophilic surface transformation. Particularly, the maximum extrema in spectral dependence of the efficiency of photoinduced hydrophilic conversion correspond to the energies of the first indirect and first direct electronic band-to-band transitions in TiO_2. At the same time, temperature dependence and the effect of the surface acidity on the hydrophilic behavior of the TiO_2 surface demonstrate the importance of the multi-layer hydrate structure in both the original hydrophilicity of the surface and the direction of the photoinduced hydrophilic conversion. Estimation of the surface energy alteration under photoexcitation suggests that

only specific surface sites (10^{-3}, 10^{-4} monolayer) are responsible for the effect of photoinduced superhydrophilicity of TiO_2 surface.

Meanwhile, the vast majority of studies on this matter have suggested that the surface photoinduced hydrophilicity is dictated by the structural changes of the water multi-layer at the surface of metal oxides. In our previous works on study of hydrated TiO_2 and ZnO coatings we have proposed following mechanism of the primary photoexcitation processes responsible for both photostimulated adsorption and photoinduced transformation of surface into new hydrophilic state:

$$S(S^+) + h(e) \rightarrow S^+(S) \quad (1)$$

$$S^+(S) + e(h) \rightarrow S(S^+) \quad (2)$$

$$H \rightarrow S(S^+) \quad (3)$$

$$S^+(S) \rightarrow H \quad (4)$$

The determinative step is a generation of photoholes (h) and photoelectrons (e), which can be trapped by the hole (S) and/or the electron (S^+) surface sites responsible for hydrophilic conversion (photoactivation) (1). There are also photodeactivation (2) and non-photostimulated deactivation (4) of these active surface sites (S^+ or/and S). The step (3) corresponds to the conversion of the surface into a new hydrophilic state (H).

It would be very useful to determine which type of photocarriers, photoholes or/and photoelectrons, rules the photoinduced hydrophilic conversion on surface of certain material. In turn, knowing this type one can predict and create the surface with proper hydrophilic properties under light. To form of the heterojunction structures comprising TiO_2 and other narrow bandgap semiconductor material (ZnO, CdS, WO_3) and to study the photoinduced hydrophilic transformations for these TiO_2-topped surfaces of formed structures under light of different spectral com-

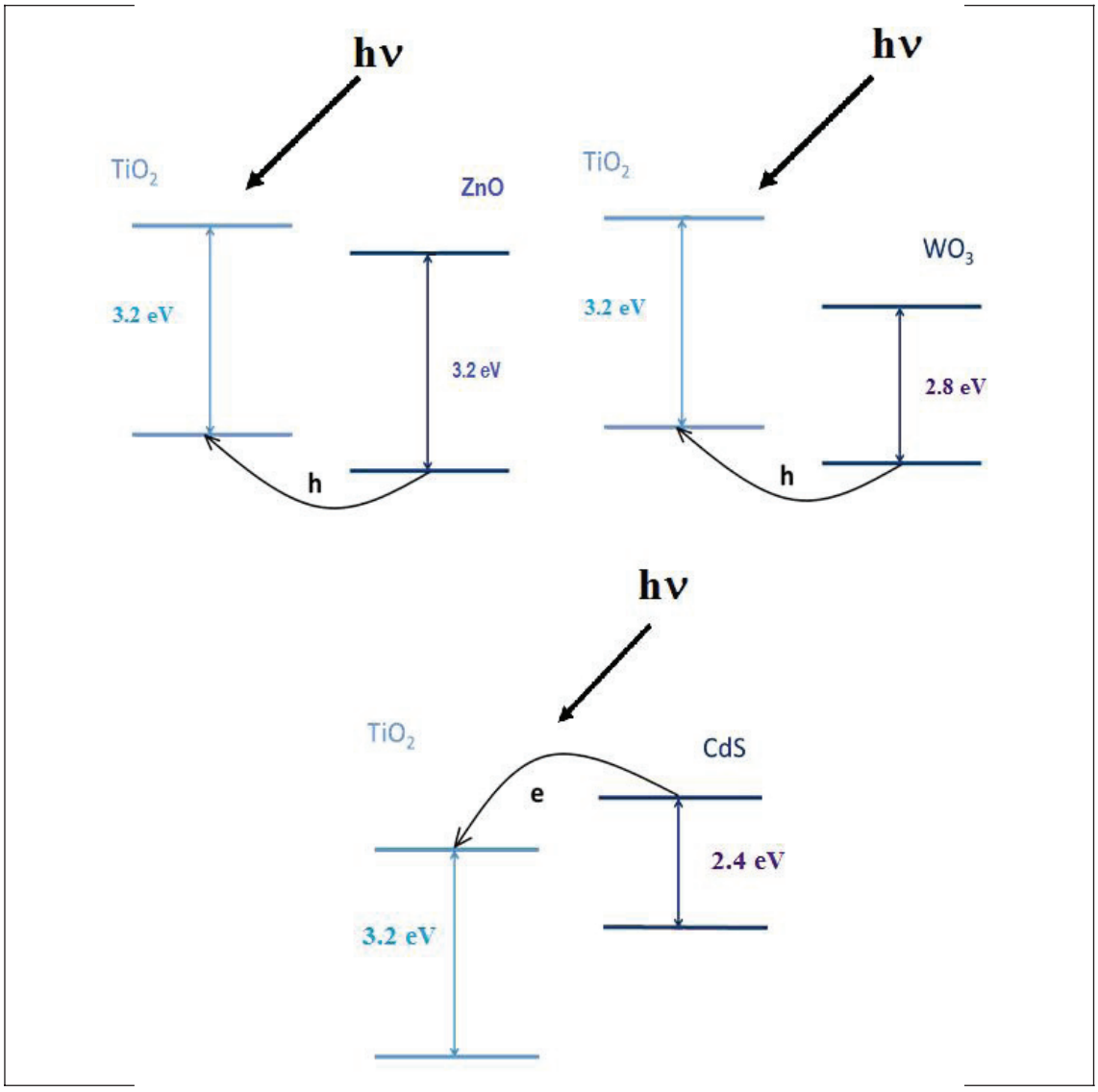

Figure 2. Schematic illustration of photoinduced electron transfer in TiO_2/ZnO, TiO_2/CdS, TiO_2/WO_3 heterojunctions.

position seems to be promising way to figure out the mechanism of photoinduced hydrophilic transition and to control the wettability of solids' surfaces.

Several strategies to improve the efficiency of photocatalytic and self-cleaning properties are demonstrated. One of these is to create composite films. Figure 2 illustrates the photoinduced electron transfer in heterostructures at the photoexcitation in intrinsic absorption region of titanium dioxide.

It is seen that in these cases there is a domination of photoholes at the surfaces of the TiO_2/ZnO and TiO_2/WO_3 systems while the surface of the TiO_2/CdS heterostructure should be possessed of photoelectrons. Moreover, irradiation of layered heterojunctions by visible light (intrinsic absorption region of cadmium sulfide and tungsten oxide (VI)) is supposed to lead to charge separation, and therefore, to increase photoelectrons or photoholes on the TiO_2-topped surfaces of TiO_2/CdS, TiO_2/WO_3 heterojunctions, respectively.

Another topic concerning self-cleaning nano-coating is to real time manipulation of hydrophilic/hydrophobic properties of semiconductor-based nano-coating surfaces. It can be caused by different factors. Photoinduced hydrophilic conversion is a promising way to do this. In recent years many works are aimed at finding a method of controllable switching between hydrophilicity and hydrophobicity of the surface. The hydrophilic surface state is generally determined by its energy. The surface energy changing can be realized in several different ways. Here we report the ability to control the surface wettability of zirconium dioxide nano-coatings by changing the composition of actinic light. Such unique photoinduced hydrophilic behavior of ZrO_2 surface is ascribed to the formation of different active surface states under photoexcitation in intrinsic and extrinsic ZrO_2 absorption regions. The sequential effect of different actinic lights on the surface hydrophilicity of zirconia is found to be repeatable and reversibly switchable from highly hydrophilic state to more hydrophobic state. Observed light-controllable reversible and reproducible switching of hydrophilicity opens new possible ways for the application of the ZrO_2 based materials.

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Computational chemistry, planetary science

SCIENTIFIC ORGANIZATION

Moscow Institute of Physics and Technology

ABSTRACT

The C-H-O system represents the backbone of organic chemistry and is of key importance to planetary science. We have explored the C-H-O phase diagram up to 400 GPa by means of the powerful evolutionary algorithm USPEX combined with a high number of density-functional calculations. Unexpected chemical phenomena were uncovered (e.g. exothermic CO_2+H_2O reactions and the formation of an inclusion compound displaying the highest stability pressure known so far for these kinds of crystals) and will be presented in this contribution.

KEYWORDS

High-pressure chemistry, computational chemistry, chemical bonding, planetary science.

ACKNOWLEDGEMENTS

This work was supported by the grant of the Government of the Russian Federation (No. 14.A12.31.0003). We acknowledge the use of supercomputer "Lobavchevsky" of the State University of Nizhny Novgorod (Russian Federation) and of the Rurik supercomputer of our laboratory at MIPT.

SUMMARY

The dramatic influence of high pressure (tens or hundreds of GPa) on reactivity is nowadays experimentally well established[i]. Crystal structure prediction approaches have become very effective in correctly anticipating experimental outcomes [ii]. Among the numerous applications, these techniques have been widely exploited to predict high-pressure reactions [iii],[iv],[v]. Composition-pressure phase diagrams

can be built by comparing the free energy (which at T = 0 K reduces to enthalpy) of the most stable structures of elements and compounds at various pressures, in order to single out the thermodynamically stable compositions. The latter are defined as those compounds for which no exothermic decomposition reactions exist. In most cases, binary phase diagrams are targeted, for the high number of possible stoichiometries in a ternary phase diagram makes its *ab initio* exploration very computationally demanding.

The C-H-O ternary phase diagram at high pressure is of paramount interest for planetary science. H_2O and CH_4, not necessarily in their intact molecular forms, are among the major constituents of giant planets such as Neptune and Uranus, where pressure can reach values of hundreds of GPa [vi]. Moreover, large icy satellites (*e.g.* Ganymede, Callisto and Titan) [vii] and comets [viii] all contain water ice, mixed with a number of volatiles such as CH_4 and CO_2, experiencing pressures up to a few GPa.

In this contribution, the C-H-O phase diagram is explored up to 400 GPa by means of the powerful variable-composition evolutionary algorithm USPEX [ix] coupled with periodic density-functional calculations. Thorough, unbiased searches were performed sampling all possible C-H-O compositions, and a total of more than 125000 structures, generated by the evolutionary method, were relaxed to the closest minimum-enthalpy configuration.

Besides uncovering new stable polymorphs of high-pressure elements and known molecules, we predicted the formation of new compounds. A $2CH_4$:$3H_2$ inclusion compound forms at low pressure and remains stable up to 215 GPa. So far, among the inclusion compounds, only gas hydrates were known to persist above 50 GPa [x]. Our $2CH_4$:$3H_2$ co-crystal not only sets a new upper limit for the stability of inclusion compounds in general, but also introduces a qualitative shift of views, for it broadens the classes of inclusion compounds stable at very high pressures. Carbonic acid (H_2CO_3), highly unstable at ambient conditions, was predicted to form exothermically at mild pressure (about 1 GPa). This fact opens possibilities for new synthetic pathways and has also important implications for planetary science. On top of that, we show that carbonic acid displays a remarkable high-pressure behavior, for it polymerizes (44 GPa) and reacts with water to form orthocarbonic acid (314 GPa). This unexpected high-pressure chemistry is rationalized in this contribution by analyzing charge density and electron localization function distributions, and implications for general chemistry and planetary science are also discussed.

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An expert system for the design crystalline materials

SCIENTIFIC ORGANIZATION

Samara State Aerospace University

ABSTRACT

- Development of an expert system, containing information about the correlations between the chemical composition and geometric-topological properties of crystal structures.
- Testing of the expert system for the prediction of structures 1, 2 and 3-periodic coordination polymers.
- Services Package for remote access to information stored in SCTMS databases.

KEYWORDS

Topology of crystal structures, ligands, metal atoms, Voronoi polyhedra, big data, knowledge base, data meaning.

ACKNOWLEDGEMENTS

Russian government (grant No. 14.B25.31.0005) for support as well as Prof. Davide M. Proserpio for helpful discussions.

SUMMARY

One of the main components in the design of new metal-organic frameworks are the choice of the complexing atoms and the ligands, which determine, as a rule, the topological type of crystal structure. To simplify this procedure, we have created a knowledge base about the complexing atoms “Topological Types of Atoms” (TTA) and ligands “Topological Types of Ligands” (TTL). We used as data sources information about the known crystal structures stored in Cambridge Structure Database (F.H.Allen, Acta Crystallogr., 2002, B58, 380) and Inorganic Crystal Structures Database (A.Belsky, M.Hellenbrandt, V.L.Karen and P.Luksch, Acta Crystallogr., 2002, B58, 364).

Only such crystal structures were taken into account, which satisfy the conditions listed below:

- the crystal structures contain metal atoms, and are not alloys or intermetallic compounds;
- statistical disordering of metal atoms and its environment are absent in the structure;
- if the structures were obviously erroneous interatomic distances or atomic volumes, incomplete or incorrect chemical composition of the compounds, they are excluded from consideration.

As a result, our sample contained 360,051 crystal structures with 692,924 metal atoms having 76 chemical species. The Voronoi polyhedron, the coordination figure and the chemical composition of the first coordination sphere have been calculated for all metal atoms. This information is assembled in the TTA knowledge base. To determine the shape of the coordination figure we developed and used a new algorithm based on angular fingerprints.

The knowledge base TTL stores for each ligand information about its chemical composition, the graph of interatomic bonds, the occurrence and the coordination type of ligand in the crystal structures. At present, the knowledge base TTL contains 161,887 entries.

Now we are creating for data processing in the knowledge bases TTA, TTL, TTD and TTO (A. R. Oganov, ed. (2010). Modern Methods of Crystal Structure Prediction. Berlin: Wiley-VCH. ISBN 978-3-527-40939-6) software that you need to find the rules and laws of crystal structure building. The results will be used for the design of new crystalline materials.

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Assoc. prof.

Design of isobutane-olefin alkylation process over the solid catalyst using catalytic distillation with side reaction section

SCIENTIFIC ORGANIZATION

St. Petersburg State Institute of Technology (technical university)

ABSTRACT

The purpose of this research is to analyze the efficiency of catalytic distillation and to adapt the catalytic distillation approach to alkylation of isobutane with butenes on a solid catalyst. A detailed simulations for catalytic distillation isobutane-olefin alkylation process were conducted. Various options regarding position of the reaction section and feed distribution were considered and optimal conditions determined. The scheme is designed especially for integration with butane dehydration and isomerisation processes to expand the feedstock.

KEYWORDS

Catalytic distillation, alkylation, zeolites, sulfated zirconia oxide, integration.

ACKNOWLEDGEMENTS

Work carried out in accordance with the grant №381 of the Russian Government to support research conducted under the guidance of leading research scientists at Russian institutions of higher education on the topic: “The process of alkylation of isobutane with light olefins on solid catalysts using reactive distillation technology” contract №14.Z.50.31.0013, on 03/19/2014.

SUMMARY

Liquid acid catalyzed alkylation of isobutane with butenes is widely applied process of production high octane number gasoline component. However, utilization of sulphuric and hydrofluoric acid have a number of drawbacks related to utilization of refrigerating agents, corrosion, pollution and safety. Alkylation with solid acid catalysts has potential environmental and safety advantages over conventional liquid-acid alkylation.

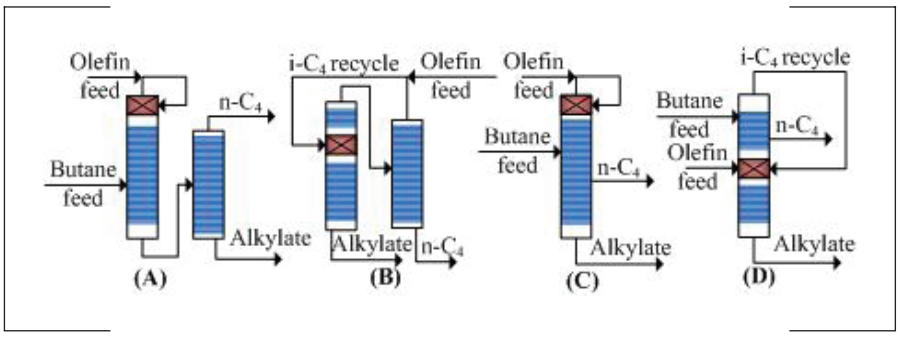
The difficulty of solid catalysts application in alkylation is related to rapid catalyst deactivation. To prevent it an excess of isobutane to olefin is required. Consequently operating costs for solid-catalyzed alkylation are increased. In order to reduce heat consumption the catalytic distillation could be proposed.

This research is focused on the special design of catalytic distillation with external reaction section for solid catalyzed isobutane-olefin alkylation and its integration with butane dehydration and isomerisation processes.

The catalytic distillation approach can provide the utilization of reaction heat. The reaction is highly exothermic (on average 75-96 kJ/mol) but the low temperature (60-100 °C) and large excess of isobutane can not be effectively utilized in the state of the art liquid-catalyzed processes.

In the reactive distillation system the process parameters (temperature and pressure) are determined by the chemical reactions, and therefore could be non-optimal for the separation. Based on experimental data the optimal conditions for alkylation with zeolitic or sulfated zirconia oxide catalysts are 60-80°C and pressure above 10 bar. The most energy demanding process, separation of isobutane /n-butane, can be optimally done at 4-7 bar. Therefore in the combined process of catalytic distillation the conditions of separation are close to the optimal. The temperature at the top of column would be close to 65 °C at a pressure level 10 bar.

Figure 1. Possible catalytic distillation design for alkylation with solid catalysts



There are several possible structures of catalytic distillation which differ in reaction and separation sections position. It

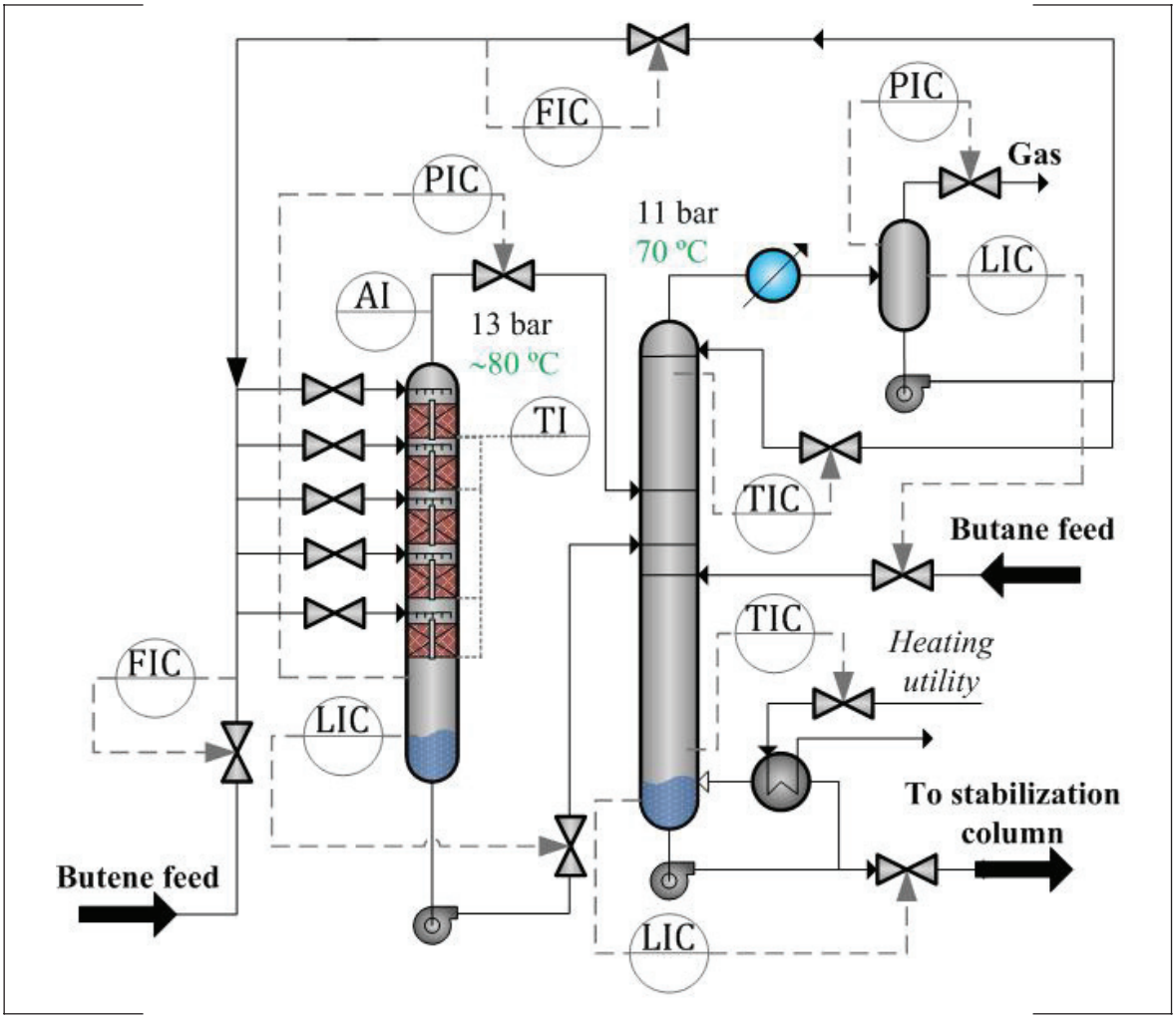
has been established in our previous research that the reaction section should be located above the butane separation zone (top of the column) and alkylate stabilization (n-butane separation) should be performed in a separate conventional distillation column (Figure 1, case «A»).

Simulations of the described processes were perfomed using Aspen Hysys. Distillation modeling was based on MESH (material balance, phase-equilibrium, mole balance and energy balance) equations approach. A set of seven alkylation reactions was simulated using conversion type equations. The simulation of the reactions were based on experimental data obtained in laboratory scale experiments for two different catalysts: zeolitic and sulfated zirconia oxide, which are considered for final design.

The traditional catalytic distillation design has a significant drawback concerning with catalyst regeneration challenge. At the current stage of solid catalyst alkylation technology, the process efficiency is mainly determined by catalyst deactivation and subsequent regeneration. In the case of severe deactivation the technological scheme should allow for continuous or semi- continuous regeneration of catalyst activity. The most promising for alkylation process is a two-step regeneration with a mild regeneration by hydrogen dissolved in liquid isobutane and subsequent regeneration with hydrogen at elevated temperature.

Therefore, for catalytic distillation the most feasible option is to have side (external) reactor sections, which number depends on reaction and regeneration time. A potential scheme of such arrangement is shown on Figure 2. Distributing the reactor is efficient method of increasing the P/O ratio on the economical basis. The temperature control of reactions can be established using different pressure of reactor and distillation column.

Figure 2. Possible catalytic distillation design for alkylation with solid catalysts



Another question, which is considered in the study, is the integration of alkylation with butane dehydration and isomerisation processes. The state-of-the-art condition of these processes are very different, but its modification, including catalyst, and single separation section utilization can be efficient and provide the extension of process feedstock by relatively cheap olefin free streams from refinery plant.

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Engineer

Ionic transport in zirconia-based single crystals

SCIENTIFIC ORGANIZATION

Institute of Solid State Physics, RAS

ABSTRACT

Materials based on zirconium dioxide have a number of unique physico-chemical, mechanical and electrical properties that determine their use in various fields, such as: medicine and technology. Solid electrolyte based on partially stabilized zirconia (PSZ) or completely stabilized zirconia (SZ) are the most popular and studied for practical use (in particular, in the solid oxide fuel cell) today. The main feature of these materials is the presence of exclusively anionic conductivity, which determines their use in SOFCs as an electrolyte membrane.

KEYWORDS

Ionic transport, ion conductors, zirconia-doped monocrystals, zirconia-based monocrystals, partly-stabilized zirconia.

SUMMARY

The main purpose of this work is to study transport properties of single crystals based on zirconium dioxide and it's dependence on the concentration of the stabilizer. For convenience, researches are carried out on single crystals, as ceramics have the grain boundaries, which, in turn, have characteristics distinguish from the bulk, as well as it have an affect on the measurment stability. Thus, the results of measurements of physical characteristics such as electrical conductivity, are related only to the volume of material and eliminate the influence of the grain boundaries, which significantly facilitate selection of composition and help evaluate the quality of products made of ceramic materials used in SOFC.

In this work conductivity of monocrystals of partially stabilized zirconia (PSZ) Zr (1-x-y) Sc (y) Y (x) O (2-z) is measured by impedance spectroscopy.The temperature dependence of bulk conductivities is constructed. The influence of overall concentration of dopants and the concentration of Y_2O_3 and Sc_2O_3 separately on the conductivity of single crystal is determin.

Sukhorukov Gleb
Professor

Remote Controlled Systems for Theranostics

SCIENTIFIC ORGANIZATION

Queen Mary University of London

ABSTRACT

The talk will review recent advanced in development of remote controllable delivery systems, where micro- and nanostructured carriers can be addressed via light, magnetic field and ultrasound resulting on their navigation and deploy of cargo at designated area

KEYWORDS

Delivery systems, polymers, nanoparticles, encapsulation.

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K+-conductive inorganic ternary and quaternary compounds as advanced materials for solid electrolyte batteries

SCIENTIFIC ORGANIZATION

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ABSTRACT

In our research all quaternary and ternary potassium-oxygen compounds KaX1bX-2cOz taken from Inorganic Crystal Structure Database (ICSD) were analyzed for the first time. By means of the Voronoi-Dirichlet approach, implemented in program package ToposPro, migration paths of K^+-cations for selected structures were calculated and we found 179 compounds containing 1D, 2D and 3D migration maps, which were not considered earlier as possible potassium-conductive electrolytes.

KEYWORDS

Crystallochemical analysis, cation conductivity, Voronoi-Dirichlet approach, free migration.

ACKNOWLEDGEMENTS

The author is grateful to V.A.Blatov and N.A.Kabanova for their valuable recommendations.

SUMMARY

A challenge for the materials science is the search for alternative cation-conductive materials, in particular, potassium- or sodium-conductive solid electrolytes, which can be used to create new prospective chemical sources of energy. One of the solutions of this problem is the processing of large amounts of structural data by means of special software based on modern methods of crystallochemical analysis.

The geometry of the migration channels is an important factor which determines the prerequisites for cation conductivity in the structure. In [1, 2], the promising lithium and sodium oxygen-containing compounds, possessing 1D, 2D, or 3D infinite systems of channels (the migration maps) available for Li^+ and Na^+-cations respectively, have been found basing on the Voronoi-Dirichlet approach.

In this work, we have analyzed all known ternary and quaternary potassium-oxygen-containing compounds (2729 compounds) from the Inorganic Crystal Structure Database (ICSD version 2015/1). The systems of voids and channels were found in the selected structures using the Voronoi-Dirichlet approach, which is implemented in the ToposPro program package [3]. In total, 232 compounds were found, whose structures allow free migration of potassium ions. Out of the 232 compounds, 53 substances are known as K^+-solid electrolytes, while the remaining 179 compounds, which possess 1D, 2D, or 3D migration maps of K^+ cations (Fig. 1), have not been electrochemically studied so far. They can be used as precursors for the synthesis of new potassium-conductive solid electrolytes.

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A new technique for in-situ Raman spectroscopic analysis of redox mechanisms at the solid oxide fuel cell electrodes

SCIENTIFIC ORGANIZATION

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ABSTRACT

A new technique for in-situ Raman spectroscopy uses optically transparent, single-crystal, scandia-yttria stabilized zirconia oxide membrane and special electrodes' geometry for directly observation spectra from the TPB zone. Combination of that technique with current-voltage method and impedance spectroscopy gives opportunity to study local electrochemical reactions exactly in SOFC working conditions: working temperature, separated gas chambers and current load.

KEYWORDS

SOFC, electrode, anode, Raman spectroscopy, reduction.

ACKNOWLEDGEMENTS

The authors would like to thank the Russian Foundation for Basic Research (grants 14-29- 04031 and 13-03- 12408).

SUMMARY

Solid oxide fuel cell (SOFC) is a high-effective electrochemical device which directly convert chemical energy of fuel and oxidizer in electrical and thermal energy. Effectiveness of SOFC is strongly dependent on the kinetics of the electrode redox reactions which take place at the "electrode | electrolyte" interface. Traditional electrochemical techniques of reaction studies are impedance spectroscopy and current-voltage measurements. Current-voltage method is cumulative, and doesn't give enough information about chemical reactions in SOFC electrodes.

Impedance spectroscopy uses simplified processes' models for interpretation of the unclear and doubtful results obtained. One of possible techniques without these drawbacks is Raman spectroscopy. The Raman spectroscopy is widely used to investigate both cathodic and anodic processes in SOFC. Previous Raman spectroscopy studies of SOFC obtained results from and mainly related to outer boundaries of the model electrochemical cells, primary electrode surface. The most interesting point of the electrode system is "electrode | electrolyte" interface, where the electrochemical reaction take place, it cannot be accessed looking at surface and edge areas. This is because the laser excitation radiation has low penetration depth (near 1 um). To avoid that problem in the present work optically transparent, single-crystal, scandia-yttria stabilized zirconia oxide membrane was used. Electrodes of special geometry make possible to directly observe Raman spectra from the TPB zone.

A new technique described in that article also uses a traditional impedance spectroscopy and current-voltage methods. This combination of experimental techniques gives opportunity to study local electrochemical reactions exactly in SOFC working conditions: working temperature, separated gas chambers and current load. Present work is focused on the results of in-situ investigation of redox reactions in anode electrode with usage of the new technique.

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Engineer of the first category

Quenching of quantum dot luminescence under light irradiation

SCIENTIFIC ORGANIZATION

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)

ABSTRACT

Applications of quantum dots (QDs) in optoelectronics can be limited by their stability under intensive irradiation. We have studied the stability of core/shell QD photoluminescence under the irradiation typical of the laboratory. Our results show that QD photoluminescence stability is determined by the structure and thickness of their shell. It has been shown that the observed photodegradation of QDs is basically caused by the transfer of excited charge carriers outside the QD.

KEYWORDS

Quantum dot, light irradiation, luminescence quenching.

ACKNOWLEDGEMENTS

This study was supported by the Russian Science Foundation, grant no. 14-13-01160. We thank Vladimir Ushakov for the help in preparation of the manuscript.

SUMMARY

Size-tunability of the absorption and fluorescence properties of colloidal quantum dots (QDs) makes them an attractive material for modern science and technology. Size-controllable optical properties of QDs allow their applications in multiplexed biolabeling, solar cells, light emitting diodes, catalysis, *etc*. QDs may gradually replace organic dyes from these fields because of their higher linear absorption cross-sections, photoluminescence (PL) quantum yields (QY), and photostabilities. However, in contrast to organic dyes, QDs are known to be susceptible to environmental factors such as oxygen; in addition, intense laser irradiation is known to alter their PL QY. Therefore, understanding of the mechanisms and factors causing instability of QD optical properties is one of the most important issues for the development of new generations of QDs and QD-based devices.

In this study, we have investigated the influence of long-term visible-light irradiation on the PL QY of QDs in order to model their storage and/or operation under common laboratory or industrial conditions. Two types of light sources with the same light power output (15 mW/cm^2) were used for QD irradiation: a 40 W incandescent lamp and an array of light-emitting diodes with a radiation wavelength of 405 nm. Three types of core/shell QDs with different shell compositions and thicknesses, CdSe/ZnS(3ML), CdSe/ZnS(1ML)/CdS(1ML)/ZnS(1ML), and CdSe/CdS(7ML)/ZnS(1ML), all with initial PL QYs exceeding 70%, were used to estimate the effects of the shell thickness and confinement potential on the stability of their PL. QD solutions in chloroform with an optical density at the first excitonic transition maximum of 0.1 were placed into 10-mm light path quartz cuvettes and irradiated under continuous stirring in the ambient atmosphere. Along with the irradiated samples, reference samples of the same solutions were stirred in the dark for the same time intervals.

Irradiations of QDs with an incandescent lamp and a LED array have revealed two parallel counteracting processes: an increase in and quenching of the PL. The kinetic curves of these processes are shown in Figure 1.

In the case of CdSe/ZnS(3ML) QDs, irradiation with an incandescent lamp caused a slow PL decline to 48% of the initial PL QY value, while irradiation with LEDs caused a rapid PL quenching to 52% followed by slow restoration of luminescence to 48% of the initial level.

Multishell CdSe/ZnS/CdS/ZnS QDs exhibited a similar kinetic of PL QY decrease, but the degree of PL quenching was much lower. Thus, irradiation with an incandescent lamp caused a 10% drop of PL, while irradiation with a LED array resulted in a 18% loss of PL QY followed by restoration to 90% of the initial PL QY during the remaining period of irradiation.

Thick-shell CdSe/CdS(7ML)/ZnS QDs exhibited a totally different response to irradiation with both light sources, without considerable PL quenching. These QDs

were found to be almost completely stable under long-term irradiation; under irradiation from either source, a slight general growth of PL QY to 104% of the initial value was observed. The reference samples representing the same solutions of QDs incubated in the dark did not exhibit detectable variation of PL QY, thus proving that the observed effects originated from light irradiation rather than from other possible environmental factors.

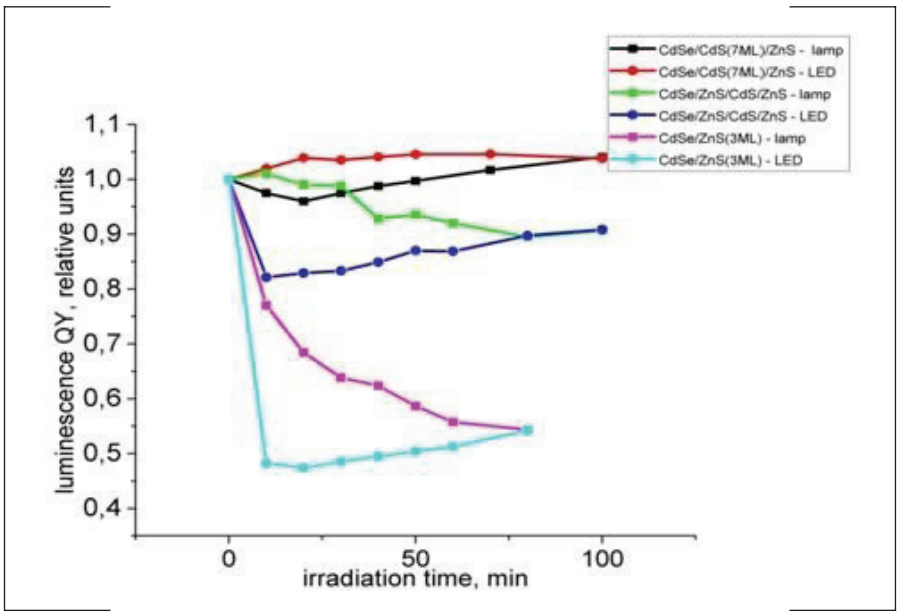

Figure 1. Quantum dot luminescence quenching under light irradiation

Transfer of the excited charge carriers from the core of QDs to the surface ligands or the surrounding molecules is known to be an efficient pathway of QD PL quenching [1]. We suppose that the difference in charge transfer rates is the reason of the observed differences in the PL quenching kinetics of the QDs studied. This difference can be related to the variation in (i) the shell thickness or (ii) the confinement potentials determined by the structure and composition of the shells. Specifically, a 3ML-thick ZnS shell ensures a high potential barrier of moderate length for electrons and holes to tunnel through and to escape the QD core. The mutishell structure provides a slightly higher potential barrier than a 3ML-thick ZnS shell does, due to the strong quantum confinement effect in monolayer-thick shell layers [2], while having the same barrier length. Finally, thick-shell CdSe/CdS(7ML)/ZnS QDs have the lowest energy of potential barrier created by CdS, but the barrier length is 2.5 times larger than that in other QDs. From the obtained results, one can conclude that the barrier length has a much stronger effect on the stability of QD colloidal solutions to irradiation, and a sufficiently thick shell could completely protect QDs from photoinduced degradation.

The difference in PL quenching kinetics under irradiation from different light sources can be attributed to different spectral overlaps of the light source emissions and QD absorption spectra. The entire incident photon flux from the blue LED array falls within the absorption range of all types of QDs, while a major part of the incandescent lamp irradiation cannot be absorbed by QDs. However, we can conclude that, even in the latter case, significant quenching of QD PL can occur under long-term irradiation.

It is noteworthy that the rate of restoration of QD PL seems to be independent of irradiation in all the three cases (Figure 1) and is likely to be caused by a different factor. Identification of this factor will be the subject of further research.

The results obtained in this work could be important for application-driven design of novel QDs. The high stability of PL QY is an advantage in engineering of photostable fluorescent biolabels or QD-LEDs; on the other hand, QDs that are prone to fast photoinduced PL quenching could be efficient tags in high-resolution stimulated emission depletion (STED) optical microscopy.

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Production of membrane-electrode assemblies for solid oxide fuel selected aspects

SCIENTIFIC ORGANIZATION

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ABSTRACT

Planar electrolyte-supported construction is one of the most promising technology of solid oxide fuel cells (SOFC) manufacture. One needs to increase the area of solid electrolyte membrane to increase the ratio of the electrochemically active area to the total area of the membrane. One of the approaches to manufacture the membrane-electrode assemblies (MEA) with large area is co-firing technique. This approach allows to compensate the mechanical stresses on different sides of the membrane.

KEYWORDS

Solid oxide fuel cells, SOFC, electrolyte membrane.

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation (Russian Federation President grant 14.W01.15.5794-MK for support of young researchers).

SUMMARY

Simultaneous decrease of the membrane thickness and increase of the membrane area do not allow to use the method of consequent formation of the electrodes, which requires the series of the high-temperature annealing at different temperatures. Those annealings lead to the deformation and even crack of the electrolyte membrane.

Earlier we reported the results of MEA manufacture by consequent firing [1] and co-firing of the electrodes at lower (<1200 °C) temperatures [2]. This work is focused on the results of MEA manufacture based on three-layered solid electrolyte membranes made by means of tape-casting technique at NEVZ-Ceramics CJSC with multilayered electrodes. Fuel cells were manufactured by means of co-firing technique at the elevated temperatures (>1200 °C). Anode electrode was made of NiO and anion conductor composite, cathode electrode was based on lanthanum-strontium manganite LSM $(La_{0.8}Sr_{0.2})_{0.95}MnO_3$) with GDC barrier layer.

This work is focused on MEA electrochemical tests: IV- and power-curves, impedance spectra.

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Creating of titanium dioxide nanocoatings with different morphology on titanium matrix for bone implants

SCIENTIFIC ORGANIZATION

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ABSTRACT

An important direction in the development of medical material science is the development of surface modification techniques that will increase osteocompatibilty of metal implants and tissues. Such materials can be used as implants in dentistry, orthopedics and traumatic surgery. In our work, the bio-active surface of titanium supports were created due to the simulation of the mesoporous structure of the titanium dioxide film and its composition, as well as the thickness of the coating in the nanorange.

KEYWORDS

Titanium dioxide film,bio-active surface, metal implant/

ACKNOWLEDGEMENTS

This work was supported by the Federal Target Program “Research and development in priority areas of Russian scientific and technological complex for 2014-2020” contract № 14.604.21.0084 (unique identification number RFMEFI 60414X0084).

SUMMARY

Nowadays, products created from different alloys began increasingly using in orthopedics. However, the use of untreated metals or its alloys can be rejected by the body. For this reason it is very important that the materials used in medicine should have biocompatible and bioactive.

Examination of a possibility of the formation of a chemical bonds between an artificial implant surface, for example titanium, and a bone tissue is one of the major characteristics of modern biocompatible materials intended for orthopedics, reconstruction surgery, and dentistry. The important problem of the chemical material science is the creation of a such dental implant surface that would be able to create rational conditions for a contact osteogenesis (formation and evolution of a bone tissue), which is the optimal mechanism for the formation of an organotypic osteal material on the implant surface. It was shown earlier that the elemental composition of the implant surface and a surface relief of a titanium play an important role as in formation of osteoblasts (young osteal cells) and in increasing of their osteocompatibility [1]. It is fair to say that qualitative and quantitative characteristics of osteointegration directly depend on surface topography of titanium implants, including nanostructured implants, and on their chemical composition [2]. Therefore the important direction for the evolution of medical material science is the development of methods of surface modification, which will make it possible to increase osteocompatibility of metal implants and organism tissues. This can be implemented by two ways to create links between the implant and the living tissue:

1) mechanical cohesion as a result of the intergrowth of tissue in the implant structure;

2) chemical interaction with the tissue components of the elemental composition of the implant;

In the work it was carried out a second way to build links between the implant and the living tissue. The bioactive surface on titanium supports were created due to the simulation of the mesoporous structure of the oxide film and its composition, as well as the thickness of the coating in the nanorange. For directional control of biomedical properties due to the structure modeling of nanometal surface sol-gel technique was used. This method allowed to obtain a mesoporous film of titanium oxide on the metal surface in the nanorange.

Also, it was solved the problem of choosing nanocoating with an optimal surface structure in the context of accelerating of osteointegration period for implants based on titanium.

In the literature, it is presented the results of works on the creation of monolithic and transparent films on substrates [2], and in the conclusions researchers usually focus their attention on the fact that they found the synthesis conditions leading to the production of continuous defect-free films. Our task was to synthesize a film having a microcrack network penetrating the whole film volume using a dip coating technique in conditions of a high thermal gradient. This a coating texture can strengthen adhesion between cells and titanium surface.

The first stage of work was the testing of synthesis techniques of the starting titanium oxide sol. As a result, we chose the method described in [3] based on the hydrolysis of titanium tetraisopropoxide in the presence of diethanolamine in isopropyl alcohol. The next step was the testing of the mode of application of the film on the model titanium substrate by dip coating method. As a result films with various thickness were obtained. For comparison of measured film thicknesses we used a theoretical model of the Landau-Levich. When the film applied to the coating by different methods, it is often important to depicture what a film will be obtained, i.e. its structure and thickness. For dip-coating method, the film thickness depends on the characteristics of the liquid adsorbent according to Landau-Levich law. The thickness of the film depends on the rate of drawing the sample from liquid, viscosity, density and surface tension. The latter also depends on the concentration of the liquid, therefore the concentration also affects the thickness of the film produced. [4]. In reality, there are deviations from Landau-Levich law, that depend on many parameters. However, considering the uncertainty, the experimental system can be described by a theoretical model of the Landau-Levich.

We have compared the theoretical and experimental results for the films with different content of titanium dioxide in the ash. As we have established a practical model differs from the theoretical hard enough. High uncertainty is taken when film thickness is measured by elipsometric method. Contribution in uncertainty is taken by surface irregularities - about 5%, and porosity - about 10%. Also, uncertainty occurs during measuring of viscosity and surface tension. With all of these uncertainties it can be said that the model of the Landau-Levich cannot describe our system yet. It was also noted that an increase in the drawing speed of the substrate from liquid increases divergence with Landau-Levich theoretical model. It can be explained that at high rates the viscous resistance induced by gravity cannot compensate the adhesion of layer [5].

For film deposition by dip-coating method drawing speed of 100 mm/min was chosen. According to electron microscopy of the cleaved film, the film had a thickness of 110 to 200 nm. Then, possibility of creating a film having a network of microcracks was explored. To solve this problem the film were obtained in the conditions of significant temperature changes and rapid drying of the precipitated gel. According to electron microscopy, a cracks passed through the entire thickness of the oxide layer at an angle close to 90°, their width was from 0.3 to 2 microns. At the same time all the cracks have been combined into a single network. It was also shown that the thickness of the film is an important factor affected on crack resistance of film, that is confirmed by other authors.

After the film deposition the samples were washed out from the organic components in the distillate water and then calcined. Scanning electron microscopy revealed that the uniformity of the coating as a result of this treatment is reduced, but not significantly.

Research of osteocompatibility of obtained samples with a TiO_2 layer was carried out in comparison with a titanium sample with its own (real) titanium oxide.

Evaluation of cell state (the character of adhesion and spreading of the cells on the pattern surface) was performed using scanning electron microscopy. Despite the fact that the cell concentration during exposure on the sample surface was the same on the surface of the titanium sample with its own (real) titanium dioxide it was detected only single cells of osteoblasts. This may reflect the low adhesion properties of the surface of the sample to the test cell line. The titanium sample with deposited titanium dioxide coating was characterized by the formation of the cell monolayer of osteoblasts on a surface with good adhesion. This indicates a high degree osteocompatibility of our coating.

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ADDITIONAL INFORMATION

Co-authors: Arbenin A.Y., Orekhov E.V., Valiev R.Z., Smirnov V.M. This work was supported by the Federal Target Program “Research and development in priority areas of Russian scientific and technological complex for 2014-2020” contract № 14.604.21.0084 (unique identification number RFMEFI 60414X0084). Form of participation: poster presentation.

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Yttrium-aluminoborate glasses containing Tb2O3, Ce2O3 and Sb2O3 for visualization of UV and X-ray radiation

SCIENTIFIC ORGANIZATION

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ABSTRACT

Yttrium-aluminoborate glasses containing Tb2O3, Ce2O3 and Sb2O3 are found to provide a full absorption of radiation with wave length less than 320 nm in layer of ~ 50-100 nm thick. They manifest an effective (up to 80%) luminescence of Tb3+ ions sensitized by Ce3+ ions as well as weak concentration quenching of luminescence. Yttrium-aluminoborate glasses are established to show high-effective green luminescence under UV and X-rays irradiation.

KEYWORDS

Aluminoborate glass, huntite, rare-earth ions, luminescence.

SUMMARY

Rare-earth (RE) doped glasses and fibers are attractive materials for applications in lighting and optical displays however they suffer from concentration quenching of luminescence resulting in low light yield. The concentration quenching occurs due to solubility limit of RE ions in oxide glass which cause segregation (clustering). Segregation takes place even at low concentrations of RE ions. Clustering facilitates energy migration between RE ions resulting in luminescence quenching due to the interaction between emission activator ions. Large distance between RE ions allows some control of the RE ions clustering. In order to suppress concentration quenching process among the doped ions and initiate intense luminescence in the glass host, searching of matrices with a large RE-RE distances is quite actual.

Among different oxide hosts with large RE-RE distance yttrium-aluminoborate crystals

$RE_xY_{1-x}Al_3(BO_3)_4$ with huntite-like structure and the distance between RE about 0,59 nm are indeed promising candidates [1]. Prevailing content of boron oxide in huntite crystals assumes high glass-forming ability of melts and possibility of production of transparent glasses with the composition identical to that in the crystals.

It has been recently shown that the structure of the huntite cation lattice is preserved by passing from $Sm_xY_{1-x}Al_3(BO_3)_4$ polycrystals to Sm-containing huntite-like glasses with RE-RE minimum distance of about 0.67 nm. It has been shown that

quantum yield of luminescence turns out to be 80% in glass in contrast to that of 55% in polycrystals due to a decrease of [BO_3] group content [2]. The presence of [BO_3] vibrational groups allows to use RE ions as activator with energy gap, DE, between a metastable state and a lower state above 8000 cm^{-1}. The energy gap between a metastable state and a lower state of Tb^{3+} ions is about 14500 cm^{-1} and of Ce^{3+} ions is about 25000 cm^{-1}. Moreover, Ce^{3+} ion shows an efficient broad band electric dipole allowed 5d-4f transition and acts as a effective sensitizer, transferring a part of its energy to various activator ions, such as Tb^{3+}. That's why yttrium-aluminoborate glasses containing Tb^{3+} and Ce^{3+} ions were selected and synthesize to study their luminescence properties.

Yttrium-aluminoborate glasses with nominal compositions (mol. %) $10(Ce_xTb_yY_{1-x-y})_2O_3$-$30Al_2O_3$-$60B_2O_3$ (x=0,9, y=0,10) were prepared by melt-quenching method. All chemicals used in the synthesis were of "chemically pure" grade. Batches were calculated to yield 20 g of glass and were mixed homogeneously in a porcelain mortar and subsequently melted in an platinum crucible at 1480 °C for about 1 h in air. The melt was pressed between two stainless steel plates and finally annealed at 660°C for 3 h followed by cooling naturally to room temperature.

Absorption spectra were recorded on UV-3600 (Shimadzu) and Varian Cary-500 (Agilent) spectrophotometers. Excitation, emission spectra and luminescence decay curves were obtained on SDL-2 spectrofluorimeter (LOMO, Russia) and by means of a pulsed dye laser (YAG:Nd^{3+}, Dt_{imp}» 10 nc) a photomultiplier and a digital oscilloscope. XEL spectra were examined using an X-ray tube BSV-21 (30kV, 7,5mA) and detector (FEU-28).

Under melting conditions mentioned above the greater part of cerium turned out to be present in the glass in non-luminescent form as Ce^{4+}. Addition of Sb_2O_3 leads to stabilization of cerium ions in triply charged state that gives rise to green luminescence under UV excitation.

It was found out that Sb^{5+} ions also take part in the Tb^{3+} ions luminescence sensitization. An attenuation of Tb luminescence occurs when the concentration of Sb^{5+} ions exceeds 1 mol. %. The explanation of this fact may be in the screening of the Tb absorption bands by the Sb^{5+} ions. A study of Sb luminescence revealed the possibility of using these glasses as quasi white phosphors.

The Judd-Ofelt intensity parameters for f-f transition of Tb^{3+} ions were determined for yttrium-aluminoborate glasses containing Tb^{3+} and Ce^{3+} (TCG) ions and containing only Tb^{3+} (TG). The following parameters were obtained: $\Omega 2 = 5.45'10^{-20}$, $\Omega 4 = 2.82'10^{-20}$, $\Omega 6 = 3.76'10^{-20}$ cm^2 for TCG and $\Omega 2 = 4.99'10^{-20}$, $\Omega 4 = 2.18'10^{-20}$, $\Omega 6 = 3.51'10^{-20}$ cm^2 for TG. Thus doping Ce^{3+} into glass as a co-activator doesn't affect the local environment of Tb^{3+} ions.

As a result glasses containing Tb_2O_3, Ce_2O_3 and Sb_2O_3 showed luminescence quantum yield up to ~80% and full absorption of UV radiation at $\lambda \leq 320$ nm in a layer ≤ 100 μm thick. The study of influence of different RE oxides on the spectrum luminescence characteristics allowed to establish that the composition $60B_2O_3$–$30Al_2O_3$–$1Ce_2O_3$–$6Tb_2O_3$+$1Sb_2O_3$ is close to optimal and that huntite-like glasses are promising for the fabrication of heavily doped active media and can be used as visualizers of UV radiation for the producing of converters of UV radiation into the yellow-green region of the spectrum.

Yttrium-aluminoborate glasses are found to show green luminescence under X-rays, and the addition of heavy elements such as Pb causes the increase of luminescence, and a high scintillating efficiency of about 30% of that of the $CdWO_4$ crystal was achieved.

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ADDITIONAL INFORMATION

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Anisotropy of intermolecular interactions and its relation to mechanical properties of organic molecular crystals

SCIENTIFIC ORGANIZATION

SCTMS

ABSTRACT

Two descriptors are proposed that can be used for description and classification of crystal structures. The first one was used for prediction of cleavage planes in molecular crystals. In all the cases cleavage planes coincided with the planes corresponding to layers with highest X value. The second proposed descriptor is more general, but both of them are needed both for systematics of molecular crystals and for the development of expert systems in materials science.

KEYWORDS

Intermolecular interactions, molecular crystals.

ACKNOWLEDGEMENTS

The work was supported by the Russian government (Grant 14.B25.31.0005).

SUMMARY

Relationship between structure and mechanical properties of molecular crystals are of great interest for many applications in microelectronics, technology of high-energetic materials and especially in pharmaceutical industry. Anisotropy of molecular forces plays a leading role in determining the solid's response on the applied mechanical stress but by now, only few schemes were proposed for description of interaction energies in molecular crystals, e.g. analysis of dimensionality if intermolecular interactions [1].

We propose two such descriptors for crystal structure – X parameter and anisotropy index (AI) – that characterize anisotropy of intermolecular interactions. The information on the strength of intermolecular interactions was obtained with the PIXEL method [2], which is suitable for these purposes because of its accuracy and relatively low demands in computational resources. The physical meaning of the first descriptor is related to intermolecular interaction energy anisotropy that is the share of cohesive energy in the given layer compared to the total cohesive energy in the cluster, representing the whole crystal in PIXEL calculations. The correlation was found between magnitude of this parameter and presence of cleavage planes in molecular crystal [3]. For instance, for primary (010) and for secondary (111) cleavage planes in b-alanine crystal, corresponding values are X(010)=0.902, X(111)=0.685, i.e. larger than X values for other crystal planes. The proposed scheme was tested on 13 crystals, which were grown and subsequently tested for its mechanical properties. In all the cases cleavage planes coincided with the planes corresponding to layers with highest X value.

The second proposed descriptor evaluates anisotropy of interactions taking into account only the first coordination shell of molecule. Its value is between zero and one and in contrast from the first descriptor this one is more general (value of the X parameter is specific for a given molecular layer). Anisotropy index can be helpful in crystal structure analysis, since new crystal structure descriptors are needed both for systematics of molecular crystals and for the development of expert systems in materials science.

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EARTH SCIENCES, ECOLOGY & ENVIRONMENTAL MANAGEMENT

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Methods for assess the socio-economic impacts of natural risks on municipal level

SCIENTIFIC ORGANIZATION

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ABSTRACT

The article proposes a methodology of assessing the socio-economic territorial systems vulnerability to natural hazards on the municipal level. For this purpose we created the integral socio-economic potential density index of the territory. Integration of this index values and the degree of natural hazards exposure to the territory (in space and time) helps to identify areas of maximum risk. In practical terms, this method can be useful in planning the territorial development; it can help to choice the optimal locations for investment projects, engineering etc.

KEYWORDS

Socio-economic potential of the territory, natural hazards, the risks, municipal level.

ACKNOWLEDGEMENTS

This work was supported by the Russian Science Foundation (Project 14-37-00038, project 16-17-00104).

SUMMARY

Relevance of this study caused by increased importance of natural hazards and their catastrophic consequences for the world (in particular Russian) population and economy.

To assess the socio-economic risks of natural hazards, we developed a group of indexes, which based on a comparison of the accumulated territorial socio-economic potential and the probability of natural hazards. At creation of methods, we relied on principle: natural hazards show their essence only in the human exploration territory. Otherwise, it can be named only as ordinary natural phenomena. According to this we first developed the concept of “density of accumulated territorial social-economic potential.” For this purpose, we considered the socio-economic characteristics of the territory outside the administrative borders (inside the administrative borders, we investigated only human exploration areas).

Testing of our methods was made on the example of a group of Russian regions (the level of municipalities). We detected zones with different levels of risk. It is allowed to select municipalities, which need more large-scale studie. As a result, we have created a series of maps and typology of municipalities. It based on a combination of two parameters: the probability of natural disasters (in our case – floods, avalanches, and mudflows) and the level of socio-economic potential. The high density of the socio-economic potential of the territory provides high prospects of development. Thus development of hazardous areas is most likely (due to limited land resources). Therefore must take account of the risks of natural hazards and the proposed method is a necessary tool for this. This methodology may be used to develop monitoring systems, programs to protect the population and economic objects, territorial planning and economic development.

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Polycyclic aromatic hydrocarbons at high pressures: oligomerization, carbonization, compressibility and thermal expansion

SCIENTIFIC ORGANIZATION

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ABSTRACT

High-pressure study of polycyclic aromatic hydrocarbons (PAHs) is extremely important for Earth and planetary science. High-pressure experiments of PAHs at temperature to 773 K revealed significant oligomerization by MALDI measurements. PAH carbonization at 1.3 – 15.5 GPa was defined at 773 – 1073 K. The PAH decomposition products consist of graphite and amorphous carbon. PAHs found in fluid inclusions in mantle-derived minerals could not be formed at mantle conditions. PAHs possess almost zero temperature effect on increasing of the unit cell volumes.

KEYWORDS

High-pressure, In situ X-ray diffraction, Raman spectroscopy, Polycyclic aromatic hydrocarbons, Oligomerization, Compressibility, Carbon

ACKNOWLEDGEMENTS

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SUMMARY

High-pressure study of polycyclic aromatic hydrocarbons (PAHs) is extremely important for modern science: Earth and planetary dynamics, meteoritics, organic and fundamental basic chemistry. PAHs are believed to be the most abundant free organic molecules in the Universe. Electron delocalization over their carbon skeleton makes them remarkably stable. PAHs play a central role in the gas phase chemistry. PAHs are supposed to be an important component of C-O-H fluid in the deep Earth. PAHs have been found in natural samples such as mantle-derived garnet, olivine, and diamond from kimberlite pipes. Naphthalene, phenanthrene, pyrene, benzopyrene, and benzoperylene were identified as the primary constituents in these inclusions. Theoretical calculations of the equations of state for heavy hydrocarbons indicate their enhanced stability in the deep Earth's mantle. In addition, PAHs were also identified in carbonaceous chondrites such as Murchison meteorite, and Antarctic Martian meteorites. PAHs-bearing carbonaceous chondrites could play a significant role to the delivery of extraterrestrial organic prebiotic materials to the early Earth.

Our high-pressure studies have been focused on the most abundant PAHs: naphthalene ($C_{10}H_8$), anthracene ($C_{14}H_{10}$), pyrene ($C_{16}H_{10}$), and coronene ($C_{24}H_{12}$). High-pressure multianvil experiments of PAHs at room and low temperatures up to 773 K revealed significant oligomerization by matrix-assisted laser desorption/ionization (MALDI) measurements of quenched products. We detected intensive signals from synthesized dimers, trimers, and tetramers of selected PAHs at 7 GPa and 773 K. Higher oligomers (up to eicosamers) were detected by MALDI, but the signal intensities of these compounds did not exceed 1% of the maximum signal. Moreover the MALDI analyses of the experimental products at higher pressure (16 GPa) and room temperature revealed the minor oligomerization of selected PAHs. The number of oligomers increased with increasing initial PAH size. Oligomer formation might occur via PAH dehydrogenation and successive fusion of the initial hydrocarbon molecules through C–C bond formation. PAH oligomerization at high pressure and temperature is extremely important for PAH chemistry in space. A range of PAHs found in meteorites, cometary comae, interstellar clouds, and planetary nebulas could be explained by high pressure (shock) oligomerization.

PAH carbonization at 1.3–4 GPa was defined at 773–973 K, at 7-9 GPa - 873–1073 K, at 15.5 GPa - 873–973 K in high-pressure multianvil experiments using *in situ* X-ray synchrotron radiation. Melting was identified for naphthalene at 727 – 730 K and 1.5 GPa. Quenched products were analyzed by Raman spectroscopy. The PAH decomposition products consist of nanocrystalline graphite and graphite at 1.3 – 4 GPa and 773–973 K, amorphous hydrogenated carbon at 7–9 GPa and 873–973 K and diamond and trans-polyacetylene lying in grain boundaries at 15.5

GPa and 973 K. Determined decomposition temperatures for PAHs at 6-7 GPa (873–1073 K) are much lower than known Earth's geotherms and subduction slab P–T profiles. Thus, PAHs found in fluid inclusions in mantle-derived garnets, olivines, and diamonds could not be formed at mantle conditions. The possible origin of these PAHs can be explained as a result of polycondensation of reduced C–O–H fluid under the influence of natural catalysts through Fischer-Tropsch type reactions upon its cooling after or at the final stages of kimberlite eruption at moderate residual pressures. The possible candidates involved in catalytic reactions could be transition metals, carbon, H_2O, and CO_2. Due to the limited temperature stability of PAHs at high pressure, proposed polycondensation of reduced C–O–H fluid could be occurred only in the pressure range of 0 – 1.5 GPa and temperature lower than 900 K.

Defined PAH decomposition parameters are extremely important for understanding the planet accretion by carbonaceous chondrites such as the Murchison meteorite. Recent shock-wave experiments revealed PAH dehydrogenation at 17.9 – 36.5 GPa and 940 – 1660 K. Therefore, assuming that carbonaceous PAH-bearing chondrites accreted on and formed the Earth, they should have dehydrogenated at a point where the growing Earth reached a radius of 1525 - 3060 km and most of the hydrogen delivered to the Earth had been discharged into the atmosphere by the end of the accretion. In our static experiments we defined that carbonaceous chondrites such as the Murchison meteorite accreted on the early Earth could not be dehydrogenated until at a point where the growing Earth reached a radius at least of 1375 - 1575 km. Further growth and the heating of the Earth led to the decomposition of accumulated PAHs to carbon and hydrogen in the interiors. However, smaller celestial bodies, also formed by the collision of meteorites, should preserved in their depths complex polycyclic hydrocarbons. Indeed, PAHs could not survive via possible heating episodes and formation of global magma oceans in the early Earth.

Recent high-pressure diamond anvil cell experiments defined compressibility curves of naphthalene, anthracene and coronene at room temperature up to 13 – 14 GPa. Our determined thermal expansion data for PAHs are consistent with the appropriate compressibility curves. We found that PAHs possess very low temperature effect on increasing the unit cell volumes at pressures 1.3 – 7.9 GPa for the temperature range of 298–873 K. Such a diminishing of thermal effects with the pressure increase is apparently a specific feature of the high-pressure behavior of molecular crystals like benzene and PAHs. This may be related to low energy of intermolecular interactions and corresponding lattice phonons, which can be easily suppressed by the applied pressure.

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Using digital elevation model, satellite and ground data to mapping of vegetation cover diversity

SCIENTIFIC ORGANIZATION

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ABSTRACT

A methodology of vegetation cover mapping based on combined GIS-based analysis of satellite imagery Landsat-8-OLY, digital elevation model, and ground observation data was developed. Maps of vegetation types and vegetation growing conditions were build using the expert knowledges. The first map is based on remote sensing classification, while the second map is constructed based on DEM classification. The proposed methodology was applied for the test site area, located in the Northern Siberia boreal forests.

KEYWORDS

Geographic Information System, Remote Sensing data, Digital Elevation Model, Vegetation Mapping.

SUMMARY

Conventional methods of forest monitoring, such as field observations and thematic mapping, are often insufficient to meet the needs of today's research tasks for

information on vast and highly heterogenic land cover fragments containing forest areas with rapidly changing boundaries. For this reason, a concept of ecosystem monitoring based on space imagery analysis combined with application of mapping methodologies, GIS, and ground data has been developed as an alternative approach over the recent decades.

We have attempted to develop a methodology to classification and mapping of vegetation cover using satellite data, digital elevation model, ground observation data and GIS.

A test site area (68° - 69° N, 88° - 89° E) was located in the Northern Siberia boreal forest.

To identify vegetation type Landsat 8-OLI images were classified by the method of maximum likelihood. In the process of images classification we obtained land cover classes: forests and woodlands, forest-bog complexes, tundra, tundra-forest complexes, bogs, stones.

To correctly classify and understand the position of any one vegetation type in a vegetation development series and to assess its current state, one needs to know a vegetation growing conditions controlling the probability of occurrence of any vegetation community type. The classification of potential vegetation growing conditions was carried out: two-layer DEM-composite (elevation above sea level and slopes) was classified using ISODATA. Land cover classes relatively similar in relief morphometric parameters were identified as geomorphological complex of vegetation growing conditions. To perform more detailed classification, we analyzed each geomorphological complex and identified sites that were homogeneous in slope. Those sites corresponded vegetation growing conditions types. The electronic layer of potential growing conditions types was created as a basis of vegetation cover mapping.

Then the expert system for classification and mapping of vegetation cover was developed using Knowledge Engineer module / ERDAS Imagine. The initial classes obtained from remote sensing data classification were distributed using a preliminary classification of growing conditions types and the associated vegetation. As a result, 16 vegetation types or their complexes were obtained.

The obtained maps reflects the diversity of vegetation cover (level of vegetation types and their complexes) and vegetation growing conditions types. They can predict the pace of regeneration succession in a range of vegetation growing conditions. Therefore, these maps can be used in the complex models of carbon balance and carbon pools estimation.

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The influence of the complexation of humic substances on the migration forms of metals in natural waters, areas of northern taiga and forest-steppe of the Tyumen region

SCIENTIFIC ORGANIZATION

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ABSTRACT

Work is devoted assessing the impact of complexation of metal ions with humic substances of natural waters on the distribution of metals into molds. Applied to published data on the values of the conditional stability constants of complexes to describe theactivity of the metal in the environment. The different approaches to the estimation of complexing ability of metal ions in natural waters, the degree of toxicity and migratory activity. The features of the chemical composition of water and foreststeppe zones of the northern taiga.

KEYWORDS

Humus, water, complex, toxic.

SUMMARY

Natural water as a complex multicomponent heterophase polydisperse systems are characterized by various forms of metal. Component interaction processes in the waters are manifold: hydrolysis, polymerization, formation of colloids and

suspensions, complex. These and many other reactions cause one of the main features of the composition of natural waters is the presence in the solution of a number of coexisting chemical forms for each component [1-8].

The chemical forms of the elements differ in the migration capacity, reactivity, stability in natural waters.

If you change the physical and chemical conditions occur metal moving from one phase to another [1-4], [6-18]. [1-4], [6-18]. Depending on the environmental conditions (pH, redox potential, amount of ligand and other factors) metals exist in different oxidation states and are included in different compounds. Furthermore, all metals in the aqueous phase tend to an equilibrium state in which the forms coexist according to their physicochemical characteristics.

Study of the processes of complexation of metals with humic substances (HS) allows to predict the proportion of dissolved and colloidal forms of metals and the level of water toxicity. Dissolved form is characteristic of metals in the environment only in unpolluted waters c low turbidity (suspended solids content of at least 5-10 mg / l) [1-4], [9]. Low pH and Eh, small amounts of of suspended matter, high HS [1-4], [10-18] promote dissolution of metals, their existence in ionic form. Ionic forms of [6-8] is the most reactive and mobile, have the greatest toxicity. Therefore, abnormally acidic water in addition to the direct negative impact is transported in large amounts, many metal ions. Cations Cr (III), for example, can be carried only in very acidic environments and are deposited at an elevated alkalinity [5], [12-18]. You can say that the acidic and weakly acidic solutions c pH <6 are favorable for the transfer of the majority of trace elements in the form of ions. Increasing the pH of the medium mainly contributes to lower mobility due to deposition, as mentioned above. Complexes of metals with HS depending on the molecular weight are dissolved and colloidal form, as indicated above, each of which is characterized by a certain degree of stability. Changing the stability of metal complexes with HS determined, firstly, the physicochemical characteristics of metal, and secondly, the qualitative composition of the organic components [12-13], third, molecular weight HS [1-4], [9].

One of the important processes that determine the migration ability of trace elements in surface waters, is the interaction of metal ions with HS treatment, which has a significant impact, both on the mobility and distribution of metal into molds.

The aim of the work was carried out theoretical calculations of finding forms of metals in natural waters of forest-steppe zone and northern taiga by the results of detailed studies of natural water chemical composition on the territory of the Tyumen region. During operation the following parameters were used: the content of metal ions, the amount of water of organic matter, pH, content of inorganic anions. In the calculation takes into account the flow of competitive reactions, material balance and electroneutrality of the system. Data on conditional constants of metal complexes with humic substances were used in [18], taking into account the specifics of humic substances.

Results and its discussion. Each natural water body is an individual chemical system in which multiple factors influence the form of metal finding. The presence in the systems of inorganic anions and cations effect on the complexation process with HS, through the course of competing reactions. Analysis of the published data, and we have obtained experimental and calculated results showed the influence of the functional characteristics of different soil humic substances in the form of metal finding.

Natural waters of the northern boreal forest are characterized by lower levels of pH and total alkalinity than water-steppe zone, which affects the distribution of metals prone to hydrolysis. These include aluminum, copper, nickel. Also this fact affects the formation of the carbonate complexes of alkaline earth metal ions. If the natural waters of the forest-steppe zone of much of the alkaline earth metal is connected to the carbonate complexes, the waters of the northern boreal forest are more common form of metal ion is located. According to our data, strontium, as the representative alkaline earth metal ion is in the form of natural waters in these zones. Low concentrations of alkaline earth metals in natural waters zone northern boreal forest (Table. 2) in the presence of high (> 100 mg / l) of aluminum and iron concentrations contribute to the low binding of calcium and magnesium ions with humic treatment substances, especially if they contain organic compounds of less than 10 mg O / l.

The ions Fe (III) and Al (III) are found in high amounts (more than 100 g / L), and natural waters of northern boreal forest and steppe natural waters zone. It is worth noting the high degree of binding iron ions with humic substances in all of the investigated object. Al (III) ion is less studied, that does not allow you to compare the

results obtained with the works of other authors. It is known that Al (III) ions are able to form complexes with HS par with ions Fe (III) [6-8], but due to the diverse chemical composition of water bodies with the degree of binding of HS can vary greatly.

For example, in natural waters grove belt zone differences between the aqua ions and complex forms of Al (III) constitute more than 50-70%. Low concentrations of ions of copper, zinc and lead (less than 2 mg / L) in natural water areas forest-steppes on the rule of Le Chatelier cause predominantly aqua ions type of migration of metals, but in natural objects zone of northern taiga the degree of binding of copper ions with humic substances waters reach 20%. Cadmium in natural water areas of northern taiga and steppe is in the ionic form, which is facilitated by the low conditional constants ustoychivostikompleksov [18] and low levels of cadmium in natural waters. The complexation of nickel ions in individual water bodies of the steppe zone and northern boreal forest at low competitive environment and quantities of humus more than 10 mg O / l up to 70%, due to the low competitiveness of the humic substances in the given object. Mn (II) in natural waters Tyumensky region is in ionic form, due to low stability constants of metal complexes, and small concentrations.

Cr (III) in natural materials is advantageously in the form of hydroxil and practically does not form compounds of humic substances with water. Analyzing the form of metal finding, we may conclude that a large variability in the forms of distribution of metals in natural waters, which are determined by the composition and concentration of trace elements, especially humic substances. The chemical properties of HS in natural waters depends, in turn, on soil properties, located in the catchment area and therefore have a zonal specificity. Based on the distribution of metals in forms hazardous properties of such metals as aluminum, iron, copper occur in natural waters with low humus high total alkalinity. The toxic properties of cadmium, lead, nickel, zinc occur in the presence of large amounts of iron ions, copper, aluminum, i.e. in the presence of strong competitor's system complexation with humic substances.

There are complex mechanisms for binding and distributing forms of metals in natural waters, which are determined not only by the properties of metal ions as the overall chemistry of the water, including the entire range of metal content, as well as individual quality characteristics of humic substances. Each water system has a unique set of chemical components and HS. Physical and chemical properties of metal ions, their content, as well as the concentration of cations and anions caused specific trends in metal migration.

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Chemical and Physical Properties and Composition of the Earth's Core

SCIENTIFIC ORGANIZATION

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ABSTRACT

We conducted high-pressure mineral physics studies of the Earth's central regions. The amounts of light elements in the core are the key to clarify the formation of the Earth. We made high pressure experiments on the phase relations, compression, and sound velocity measurements. Our results on the equation of state and the sound velocity of solid and liquid iron and iron–nickel alloys strongly suggest that the core contains light elements to reduce both density and sound velocity.

KEYWORDS

High Pressure, Core, phase relation, compression, sound velocity, partitioning.

SUMMARY

We conducted high-pressure mineral physics studies of the Earth's central regions. The amounts of light elements in the core are the key to clarify the formation process of the Earth. We made high pressure experiments on the phase relations, compression, and sound velocity measurements of the iron-light element systems.

Sound velocity is the most accurate information in seismology and can provide important clues on the structure and composition of the core. In spite of its importance, the sound velocity data of the core materials at high pressure and temperature are still very limited due to technical difficulties. Recent seismological studies revealed that inner core shows seismological anisotropy together with internal structure of the inner core, such as inner-most inner core. There are debated matters also on the structure and composition of the inner core, i.e., inner core might be hexagonal close-packed iron (hcp) or body-centered cubic (bcc) structure.

We measured the compressional velocity of hcp-iron and the other alloys by the inelastic X-ray scattering (IXS) method using DAC at high pressure and temperature. Inelastic X-ray scattering spectra were taken at BL35XU, Spring-8. We made the IXS measurement to 174 GPa, the highest pressure at room temperature in this method [1]. Compressional velocity measurements at high temperature were made by using both external heating and laser heating [2]. We developed a portable laser heating system and successfully measured the IXS spectra to temperatures up to 3000 K at 163 GPa.

Measurements of sound velocities in metals at Mbar pressures, with specific focus on the compressional sound velocity of hcp-iron were reviewed [3]. A critical comparison of our results [1] and literature results, coherently analyzed using consistent metrology (pressure scale, equation of state), allows us to propose reference relations for the pressure and density dependence of the compressional velocity of hexagonal close-packed iron at ambient temperature. This provides a key base line upon which to add complexity, including high-temperature effects, pre-melting

effects, effects of nickel and/or light element incorporation, necessary for an accurate comparison with seismic models, and ultimately to constrain Earth's inner core composition.

Hexagonal close-packed iron (hcp-Fe) is a main component of Earth's inner core. The difference in density between hcp-Fe and the inner core in the Preliminary Reference Earth Model (PREM) shows a density deficit, which implies an existence of light elements in the core. We measured the compressional sound velocity (VP) of hcp-Fe up to 163 GPa and 3000 K using inelastic X-ray scattering combined with a laser-heated sample in a diamond anvil cell [4]. We propose a new high-temperature Birch's law for hcp-Fe, which gives us the VP of pure hcp-Fe up to the core conditions. We find that Earth's inner core has a 4 to 5% smaller density and a 4 to 10% smaller VP than hcp-Fe. Our results demonstrate that components other than Fe in Earth's core are required to explain Earth's core density and velocity deficits compared to hcp-Fe. Assuming that the temperature effects on iron alloys are the same as those on hcp-Fe, we narrow down light elements in the inner core in terms of the velocity deficit. Hydrogen is a good candidate; thus, Earth's core may be a hidden hydrogen reservoir. Silicon and sulfur are also possible candidates and could show good agreement with PREM if we consider the presence of some melt in the inner core, anelasticity, and/or a premelting effect.

Inner core was crystallized from the outer core. The light elements contents of the inner and outer core must be controlled by the element partitioning between the liquid and solid iron alloy, i.e., outer and inner cores. We call it the inner core fractionation. The phase relationships and the crystallization temperatures in the Fe-S-Si system were determined up to 60 GPa and the Fe-S system up to 120 GPa [5] using a laser-heated diamond anvil cell combined with X-ray diffraction technique. On the basis of X-ray diffraction patterns, we confirmed that hcp/fcc Fe-Si alloy and Fe3S were stable phases under subsolidus conditions in the Fe-S-Si system. Because of dissolution of silicon into iron, the boundary of fcc and hcp phase shifts towards higher pressure compared to that of pure iron. Both solidus and liquidus temperatures are significantly lower than the melting temperature of pure Fe and increases with pressure in this study. As compared with the slope of the present Fe-S-Si liquidus and temperature profiles of the core of planets, inner core crystallization of the Earth occurred at the bottom of the liquid outer core whereas the crystallization of the Martian core must begin at the core-mantle boundary of the Mars.

We made an experimental study on solid–liquid partitioning in the Fe–S–Si, Fe–S–Si–O, and Fe–S–Si–O–Ni systems up to 148 GPa and demonstrated that the metallic liquid phase is relatively sulfur rich, whereas the coexisting hcp-Fe phase is silicon rich. Based on our partitioning data, the equation of state of solid and liquid iron alloys, and the seismologically observed density of the inner and outer cores, the total amount of light elements in the bulk core was constrained to be 7.4–9.9 wt. %.. The present results demonstrate that the present-day Earth has a sulfur-rich outer core and a sulfur depleted inner core, and the difference in light element contents creates the seismologically observed density contrast between the inner and outer cores.

The experimental results on partitioning of Si and S between the liquid and solid iron alloys and the compressional velocity data of hcp-Fe, Fe_3S, and $Fe_{0.83}Ni_{0.09}Si_{0.08}$ determined by the IXS method revealed that the PREM outer and inner cores can be accounted for by a pair of the sulfur-enriched outer core and sulfur-depleted and silicon-enriched inner core.

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Sprites in the Earth atmosphere. Numerical and laboratory modeling

SCIENTIFIC ORGANIZATION

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ABSTRACT

Sprites are one of the most interesting high-altitude discharges in the Earth's atmosphere, which are occurring in the mesosphere and lower thermosphere at altitudes from 60 to 90 km with horizontal size about 30 km. We develop axial-symmetry plasma-chemical self-consistent model to describe influence of sprites on the chemical balance of the mesosphere and optical emissions in different diapasons. We create vacuum tank with pressure difference to model sprites in the laboratory.

KEYWORDS

High-altitude discharges, sprites, mesosphere chemistry.

ACKNOWLEDGEMENTS

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Evolution of principal nonlinear patterns of global sea surface temperature in XX century

SCIENTIFIC ORGANIZATION

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ABSTRACT

In the report we will consider the empirical method of observed spatially-distributed data expansion into principal nonlinear dynamical modes holding the dynamical properties of the system. This method applied to HadISST1 global sea surface temperature dataset on the 1870-2014 years interval provides low-dimensional modes which resolve annual cycle and large-scale patterns reflecting El Nino Southern Oscillation variability and decadal transitions of Pacific Decadal Oscillation.

KEYWORDS

Empirical modeling, principal nonlinear modes, climate, teleconnections.

ACKNOWLEDGEMENTS

The study is supported by Government of Russian Federation (agreement #14. Z50.31.0033 with the Institute of Applied Physics of RAS).

SUMMARY

1. Method of principal nonlinear dynamical modes extraction from observed spatially-distributed data is suggested.

2. The main modes of global sea surface temperature hold annual cycle, ENSO variability, evolution of PDO pattern, and also can track the evolution and possible critical changes of climate teleconnections.

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Hydrological model of Amur River basin: development and application for flood risk management

SCIENTIFIC ORGANIZATION

Water Problems Institute of RAS

ABSTRACT

The first regional process-oriented model of runoff generation for the whole Amur River basin has been developed. The model is based on the ECOMAG and a hydrodynamic MIKE-11 model. The model has been tested by hydrometeorological observations for multi-year period, including disastrous flood of 2013. Opportunities of the model have been demonstrated for solving the following problems: (1) assessing flood control effect of the reservoirs and (2) assessing hydrological consequences of climate change in the Amur basin, including climate impact on hydrological extremes.

KEYWORDS

Hydrological modeling, Amur River, climate impact, human impact.

SUMMARY

The first regional process-oriented model of runoff generation for the whole Amur River basin has been developed. The model is based on the ECOMAG modelling system and describes processes of snow accumulation and melt, soil freezing and thawing, water infiltration into unfrozen and frozen soil, evapotranspiration, thermal and water regime of soil, overland and subsurface flow. To simulate channel flow a hydrodynamic MIKE-11 model has been coupled with the ECOMAG. The model has been calibrated using streamflow discharges measured in 15 different gauges of the main river and its tributaries for 10 years (1994-2003). Validation of the model has been carried out for next 10-year period (2004-2013). On the basis of the numerical experiments, opportunities of the model were illustrated by the example of the assessing the flood control function of the existing and projected reservoirs on the Zeya and Bureya rivers. It has been shown, particularly, that the absence of the Zeya and Bureya reservoirs would have resulted in a rise of water level in the Middle Amur by 1.7–2.1 m during flood wave rise and by 0.4–0.5 m during flood peak. In this case, the duration of water level standing above flooding level could increase 2–3 times. Thus, in the absence of the Zeya and Bureya reservoirs, the after effects of the flood of 2013 in the basin of the Middle Amur could have been much more disastrous, and the damage could have been more catastrophic. In addition, hydrological consequences of climate change in the Amur basin, including climate impact on hydrological extremes, have been assessed on the basis of numerical experiments with regional hydrological and ensemble of global climate models. It has been shown that the projected hydrological changes are insignificant in comparison with the uncertainty noise.

ADDITIONAL INFORMATION

Co-authors of the presentation are: Yuri Motovilov, Andrey Kalugin.

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Freezing Precipitation and Freezing Events over Northern Eurasia and North America

SCIENTIFIC ORGANIZATION

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ABSTRACT

The issue of near 0°C precipitation is linked with several hazardous phenomena including heavy snowfall/rainfall transition around °C; strong blizzards; rain-on-snow events causing floods; freezing rain and freezing drizzle; and ice load on infrastructure. In our presentation using more than 1,500 long-term time series of synoptic observations for the past four decades, we present climatology and the empirical evidence about changes in occurrence, timing, and intensity of freezing events over most of the extratropics.

KEYWORDS

Freezing rain, freezing drizzle, precipitation.

ACKNOWLEDGEMENTS

The work was supported by the Ministry of Education and Science of the Russian Federation (grant 14.B25.31.0026) and by the NASA Land Cover and Land Use Change (LCLUC) Program (grant NNX15AP81G).

SUMMARY

Near 0°C precipitation events are widespread and may represent/create natural hazards; their frequency and intensity are changing in contemporary climatic changes, and these changes are not yet well understood and/or documented

Automation (where it was introduced) and temporal paucity (e.g., 3-h. versus 1-h. reports) affect the homogeneity of reporting of freezing events (especially, for freezing drizzle and intense freezing events). Three-hourly reporting (e.g., in the Russian Federation) seriously underestimates the daily frequency of freezing events.

Using more than 1,500 long-term time series of synoptic observations for the past four decades, we present climatology and the empirical evidence about changes in occurrence, timing, and intensity of freezing rains and freezing drizzles America, most of Europe, Russia, Belarus, and Kyrgyzstan and their changes in the past decade.

The regions with the highest frequency of freezing rains (from 3 to 10 days per year) reside in the northeastern quadrant of the conterminous United States and adjacent areas of southeastern Canada south of 50°N, over the south and southwest parts of the Great East European Plain, and Central Europe. The frequency of freezing drizzle exceeds the frequency of freezing rain occurrence in all areas.

During the last decade, substantial changes in the annual freezing rain occurrence were found:

- On the southern edge of our study domain (southeastern U.S., Central Europe, southern Russia) the frequencies of freezing events decreased along with the duration of the cold season;
- In the Arctic (Norway, north of North America, some taiga areas in Russia) and at high elevations (The Tian Shan Mountains), they “followed” the expansion of the short warm season;
- Changes in the occurrence of freezing drizzle were estimated only for Russia. We found a statistically significant nationwide decrease in this element.

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Organic matter in permafrost soils: storage, turnover and possible effects of global warming

SCIENTIFIC ORGANIZATION

Institute of Soil Science, Leibniz University, Hannover

ABSTRACT

Permafrost soils are the largest terrestrial sink for non-fossil carbon. We assessed organic matter in Siberian permafrost soils under the aspect of climate change. On about 80 soil profiles along an east-west and a north-south transect, organic carbon stocks were quantified and organic matter decomposition, stabilization and vulnerability was investigated by a range of biogeochemical methods. Results suggest large future organic carbon losses in northern permafrost soils developed in aeolian sediments, while soils of the Siberian trapp plateau may even be carbon sinks.

KEYWORDS

Climate change, lignin decomposition, permafrost soils, priming effect, soil microbial community, soil organic carbon, soil organic matter decomposition, soil organic matter stabilization,, soil minerals.

ACKNOWLEDGEMENTS

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SUMMARY

Introduction

Permafrost soils cover about 22 million km^2 in circumarctic polar areas, and 65% of the land area of the Russian Federation is underlain by permanently frozen soils. Estimates on the organic carbon storage in permafrost soils range from about 1.000 to 1.700 gigatons. With that permafrost soils are currently the largest terrestrial sink for non-fossil carbon, and small changes in the stock of organic carbon in permafrost soils will have profound impact on the atmosphere's CO^2 (and CH^4) concentration and with that very likely on the Earth's climate.

Whether these soils will become a major source of greenhouse gases in the future depends on the accessibility of organic compounds to the decomposer community under the given environmental conditions. In permafrost soils, primarily low (frozen) temperatures and high moisture is most decisive in limiting biodegradation of organic matter. Permafrost thaw will change these conditions with increasing temperature and oxygen availability likely favor conditions for microbial decay of organic matter. With this respect it is important to know whether other processes than freezing and anaerobiosis will lead to the stabilization of organic matter in permafrost soils. From temperate soils we know that the formation of mineral-organic associations by sorption of dissolved organic matter to reactive soil minerals like iron oxyhydroxydes or coprecipitation of dissolved organic matter with metal cations is a very efficient process in the stabilization of organic matter in soils. Nothing is known whether such process is relevant also in permafrost soils, and whether this may help to reduce to organic carbon losses from permafrost soils at permafrost thaw.

The goal of our work was to assess the organic matter resource in Siberian permafrost soils under the aspect of climate change with respect to the following questions:

1. What is the variability of organic carbon stocks in Siberian permafrost soils at landscape scale and within the soil profile?
2. What is the chemical composition of organic matter in permafrost soils and how is soil organic matter transformed?
3. Is organic matter stabilized in permafrost soils also by other processes than freezing and anaerobiosis and is this relevant with respect to mitigation of the consequences of permafrost thaw?

Materials and Methods

For our studies we have chosen two transects. One transect covers tundra sites with continuous permafrost from east (Cherskiy), central (Ary-Mas, Logata), and western (Tazovskiy) Siberian north. The other transects stretches in the central part of Siberia from the north under tundra vegetation (Ary-Mas, Logata) to the forest tundra (Igarka) and taiga (Tura, Baikit) further south. The sites at Igarka and Baikit are characterized by discontinuous permafrost. While the northern permafrost soils developed mostly on aeolian sediments, the soils at Tura and Baikit formed in igneous rocks (trapp basalts). In total we dug about 80 soil profiles, analyzed them for organic carbon and nitrogen contents and stocks and measured for most of the soils other general soil parameters like soil texture. On selected soil profiles, we performed some in-depth analysis of the composition and the function of the soil organic matter and the microbial community. This includes

1. density fractionation of soil and organic matter to separate different functional pools,
2. chemolytic analysis of the most prominent organic matter constituents lignin and polysaccharades to identify decomposition pathways of soil organic matter,
3. general characterization of the organic carbon using ^{13}C nuclear magnetic resonance spectroscopy as a complementary method to identify decomposition pathways,
4. quantification of bacterial, archaeal and fungal SSU rRNA genes by quantitative PCR to assess microbial community composition,
5. priming experiments in order to assess the possible role of easy available carbon and/or nitrogen source on organic matter decomposition,
6. large scale incubation experiments to delineate controlling factors on organic matter decomposition.

Results and Discussion

The organic carbon storage showed a high spatial variability of <10-50 kg m^{-2} in the soils under study. Largest stocks were observed in continuous permafrost soils developed on sedimentary parent material. Cryoturbation and cryohomogenization processes led to a large contribution of subsoil horizons (incl. the permafrost layer) to the total soil organic carbon stocks. At Igarka, comparison of permafrost soils with non-permafrost soils showed much smaller organic carbon stocks in the latter. Soils at Tazowskiy, which are characterized by very thick active layer or lacking permafrost, revealed the smallest soil organic carbon stocks. This indicates that in the northern soils developed from sedimentary materials permafrost thaw leads to prominent organic matter losses. The situation is a bit different in the soils at Tura and Baikit, which developed from igneous rocks. There, differences in organic carbon stocks between permafrost soils and soils with deep active layer or no permafrost were small, and in some cases non-permafrost soils contained even more organic carbon than permafrost soils. Hence, permafrost thaw in the large central Siberian regions may have completely different consequences than in the Siberian north. The density separation revealed that on average 56% of the organic matter in the investigated permafrost soils can be fractionated into the heavy fraction and thus occurs in form of mineral-organic associations. This may impose a possible protection mechanism against organic matter decomposition, which will be discussed later.

Even though environmental conditions are not favorable for organic matter decomposition in permafrost soils, different proxies revealed an increasing decomposition of organic matter with increasing soil depth. This is already indicated by the increasing carbon-to-nitrogen ratio along with increasing $\delta^{13}C$ ratios with soil depth. Also ^{13}C nuclear magnetic resonance spectroscopy shows a decrease of O-alkyl carbon along with an increase in alkyl carbon and aryl carbon with increasing soil depth, being indicative of a pronounced organic matter decomposition and enrichment of more refractory organic matter constituents. The chemolytic data revealed some interesting differences in the decomposition pattern of lignin and lignocellulose. In contrast to temperate soils, particularly the permafrost soils with high permafrost table and large storage of organic matter are characterized by a restrained lignin decomposition, as is indicated by constant acid-to-aldehyde ratio of the vanillyl units and rather increasing proportion of lignin-derived organic matter with soil depth. In soils with thicker active layer, more aerobic soil conditions, and smaller organic carbon stocks, lignin decomposition is much more proceeded. The restrained lignin decomposition indicates a major mechanism of organic matter sequestration in permafrost soils, which is similar as in bogs. Also similarly to

bogs, changing environmental conditions and better aeration with permafrost thaw fosters primarily losses of lignin with soil organic matter decomposition.

In the laboratory, the soils were subjected to a range of incubation experiments. Using a ^{15}N dilution assay to quantify the gross protein depolymerization indicated that the topsoil materials of the permafrost soils were not nitrogen limited. In contrast, the subsoil and particularly the cryoturbated pockets revealed a strong reduction of the protein depolymerization. This suggests a nitrogen deficiency as a control of the organic matter turnover in the subsoil. Priming experiments with monomeric and polymeric easily available carbon and nitrogen sources confirmed this result. In the cryoturbated pockets the addition of an amino acid or a protein strongly increased soil organic carbon mineralization, thus emphasizing the impact of low nitrogen availability on organic matter stabilization. In contrast, the mineral subsoil responded also positively to the addition of glucose or cellulose. This so-called positive priming suggests that the decomposition of organic matter in the subsoil is also carbon limited. Hence, if a changing soil environment will lead to a larger release of easily-available organic substances in the subsoil, i.e., by rhizodeposition, this may also result in losses of indigenous soil organic matter in permafrost soils.

As said above, the majority of soil organic matter in permafrosts soils is involved in mineral-organic associations, thus possessing a potential stabilization mechanism. In 120 soil samples from 24 soil profiles, mineralization of whole soil and of mineral-associated organic matter was monitored for 180 days to assess the temperature dependency and the protection of minerals for organic carbon decomposition. The incubation revealed a large active pool in the topsoil and in the permafrost horizons, while decomposition was restrained in the cryoturbated pockets. The application of linear mixed effects models revealed that the basic drivers for the bioavailability of permafrost soil organic carbon decomposition are nutrient availability, mineral protection and microbial community response.

Temperature was the principle driver of the organic matter mineralization throughout the whole incubation, however, the temperature effect strongly decreased with soil depth. As the organic matter quality decreased with soil depth (see above), this contradicts the carbon-quality-temperature hypothesis stating that the turnover of low quality organic matter is more sensitive to temperature increase than easier available organic matter. This observation can be explained by an active protection mechanism. Enzymes for decomposition can be excluded by physicochemical protection with the mineral soil matrix, causing substrate limitation to decomposers. This is process is almost independent of temperature and can attenuate the inherent kinetic properties of organic molecules. And in fact, linear mixed effects models indicated a partially strong negative effect of clay-sized minerals and pyrophosphate-soluble iron on organic carbon mineralization, thus confirming the stabilizing effect of organic matter by association with poorly crystalline iron oxides and clay minerals or by coprecipitation with multivalent cations (aluminium, iron).

Conclusions

Under future scenarios, besides higher soil temperature a better oxygen availability, higher nutrient availability and larger input of rhizodeposition at larger soil depth will stimulate organic matter decomposition, thus decreasing the soil organic carbon storage. At the other hand, warmer temperature will increase plant net primary production and thus organic matter input in soil, and dryer and more oxic conditions in the soils likely will increase the protection of soil organic matter by an increasing formation of reactive soil minerals, which both will lead to larger organic carbon stocks. Different permafrost systems may respond differently on these two contrasting processes. At the nowadays largely anaerobic permafrost soils in the north Siberian lowlands, the effects of a better oxygen availability on organic matter decomposition, particularly of lignin, as well as nutrient and carbon priming will outcompete the effects of an increasing organic matter stabilization by neoformation of reactive soil minerals at permafrost thawing. In the permafrost soils of the central Siberian trapp basalts, the situation is different. There, the soils do not contain as much organic carbon as the permafrost soils in the north due to the limitation of soil depth by the parent rocky material and the almost lacking cryoturbation processes. These permafrost soils are also better aerated and rooted. Hence, the negative consequences permafrost of thaw on organic carbon stocks at will not prevail, but rather the positive ones such as higher plant residue input and effective stabilization of organic matter by formation of mineral-organic associations due to high production of particularly iron oxyhydroxides by weathering from the iron-rich primary minerals. The soils in the large areas of the Siberian mountain ranges, which are partly underlain by permafrost, may thus be even carbon sinks in the future.

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Verification and calibration of Energy- and Flux-Budget (EFB) turbulence closure model

SCIENTIFIC ORGANIZATION

National Research Lobachevsky State University of Nizhni Novgorod

ABSTRACT

We examine and validate the EFB turbulence closure model, which is based on the budget equations for basic second moments. To demonstrate potential improvements in Numerical Weather Prediction models, we test the new closure model in various idealized cases, varying stratification from the neutral and conventionally neutral to stable running a test RANS model and HARMONIE/AROME model in single-column mode. Results are compared with Direct Numerical Simulation and Large Eddy Simulation runs and different numerical weather prediction models.

KEYWORDS

Atmosphere Boundary layers, Direct Numerical Simulation, Large Eddy Simulation, Numerical Weather Prediction models, Turbulence closures, Stratification.

ACKNOWLEDGEMENTS

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SUMMARY

We examine and validate the EFB turbulence closure model (Zilitinkevich et al., 2013), which is based on the budget equations for basic second moments, namely, two energies: turbulent kinetic energy E_K and turbulent potential energy E_P, and vertical turbulent fluxes of momentum and potential temperature, τ_i (i = 1, 2) and F_z. Instead of traditional postulation of down-gradient turbulent transport, the EFB closure determines the eddy viscosity and eddy conductivity from the steady-state version of the budget equations for τ_i and F_z. Furthermore, the EFB closure involves new prognostic equation for turbulent dissipation time scale τ_T, and extends the theory to non-steady turbulence regimes accounting for non-gradient and non-local turbulent transports (when the traditional concepts of eddy viscosity and eddy conductivity become generally inconsistent).

Our special interest is in asymptotic behavior of the EFB closure in strongly stable stratification. For this purpose, we consider plane Couette flow, namely, the flow between two infinite parallel plates, one of which is moving relative to another. We use a set of Direct Numerical Simulation (DNS) experiments at the highest possible Reynolds numbers for different bulk Richardson numbers (Druzhinin et al., 2015).

To demonstrate potential improvements in Numerical Weather Prediction models, we test the new closure model in various idealized cases, varying stratification from the neutral and conventionally neutral to stable (GABLS1) running a test RANS model and HARMONIE/AROME model in single-column mode. Results are compared with DNS and LES (Large Eddy Simulation) runs and different numerical weather prediction models.

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PhD
Researcher

Laboratory experiment on complex investigation of wind-wave interaction at the Small-Scale Air-Sea Interaction Facility

SCIENTIFIC ORGANIZATION

Institute of Applied Physics of the Russian Academy of Sciences

ABSTRACT

In frame of laboratory experiment several aspects of wind wave interaction were investigated: the air flow structure over steep water waves, flow structure in the water, the skin friction and vertical gradients of velocity fields at the air-water interface, flow velocity at the surface.

KEYWORDS

Air-sea interaction, particle image velocimetry, wind waves.

ACKNOWLEDGEMENTS

This work was supported by the RFBR grants (15-35-20953, 14-05-00367, 16-05-00839, 16-55-52025, 14-05-91767) and by project ASIST of FP7. Measurements and data processing were supported by RSF grants 14-17-00667 and 15-17-20009 respectively.

SUMMARY

Experiment was made at the Heidelberg Small-Scale Air-Sea Interaction Facility, the Aeolotron (annular wind-wave facility, 60 cm width, 2.4 m height, circumference of 27.3 m at the inner wall; water depth during experiments 1.0 m, water volume 18.0 m^3, air space volume 24 m^3). Wind was generated by two axial fans mounted into the ceiling, equivalent wind speeds up to 16 m/s.

Water surface position was captured by to independent methods: laser height system of a vertical airside laser sheet and a side camera that captured fluorescence emission from the near-surface water layer and imaging slope gauge [1] that was capturing slope images of the surface with high-speed camera above the surface and gradient underwater light source. Water surface velocity was estimated by tracking of heat markers made on a surface by an infrared laser.

Airside measurements were made by PIV technique: small high pH water droplets with fluorescent dye (pyranine) were generated by pneumatic nozzle, at the measuring area they were illuminated by laser sheet and captured through the side window by high-speed camera with a band-pass filter on its lens, blocking reflected laser light. Water in facility has low pH so only artificially generated water droplets emitted in fluorescence band and were visible at images. Underwater measurements were made in similar technique with underwater laser sheet and hydrogen bubbles, generated from electrolysis, or 20 μm polyamide particles as markers. Airside and underwater measurements were made separately but both were complemented by synchronized surface measurements. A phase averaging method [2] was used to obtain turbulent pulsation averaged velocity fields of the air flow over the water surface curved by a wave and average profiles of the wind velocity.

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ADDITIONAL INFORMATION

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SCIENTIFIC ORGANIZATION

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Water Quality formation Factors

ABSTRACT

Topic is factor analysis of the processes of water quality formation. The identification of the real relationships between the natural environment in the catchment areas of small and medium-sized water bodies (soils, rocks, vegetation, precipitation) and surface waters. Main Interest is the Establishing the degree of influence of anthropogenic factors on the quality of surface waters in various areas of development conditions, prediction transformation of water runoff and quality characteristics of rivers and lakes with climate change.

KEYWORDS

Water quality, non-point pollution, anthropogenic load, small rivers, small lakes, oil & gas production.

ACKNOWLEDGEMENTS

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SUMMARY

Estimation of the Influence of Possible Climate Warming on the Chemical Composition of Water (case study Western Siberia)

It is a well-known fact that a global temperature increase has been documented over the last decades [Climate Change, IPCC, Geneva, 2007]. The degree of climate changes observed in the past 50 years is different among regions. As was shown [Sherstyukov, 2009] for the major portion of European Russia (ER) between 1976 and 2006, the mean annual air temperature increased at a rate of 0.5–0.7°C per 10 yr. Positive trends in mean annual air temperature were also observed in Western Siberia (WS), but the respective rate is 0.1–0.4°C per 10 yr and is highly variable within the region. The most significant changes were detected in the extreme northwest of Siberia, where values of 0.5–0.8°C per 10 years were observed; statistically significant changes in the mean temperatures of summer months were also documented in the steppe zone of the trans-Ural region [Sherstyukov, 2009].

The scale of variations in the temperature field of the WS areas discussed here is consistent with global tendencies. For instance, according to [Pavlov, Malkova, 2005], the mean air temperature in the northern hemisphere increased in the 20th century by 0.6(±0.2)°C. The last period of warming began in the 1960s–mid 1970s. The air temperature increased in 1965–1995 in northern Russia by 1.1–1.2°C, whereas the global temperature rose by 0.5–0.6°C. Climate monitoring has shown that climate changes in Arctic and sub-Arctic regions occur more rapidly and lead to the most radical consequences influencing global atmospheric circulation. Table 1 (slide in the presentations) compares data on seasonal variations and observed tendencies of changes in air temperature for various regions of Russia. These data lead to the conclusion that the rate of increase in the mean annual and seasonal temperatures of WS is higher than that of other regions in Russia. According to [Pavlov, Malkova, 2005], the most radical changes are characteristic of the tundra.

The effect of possible climate warming on the chemical composition of waters has been estimated in a number of studies [Schlesinger, 1997; Battarbee et al., 2005; Skjelkvele, Wright, 1998; Alcamo et al., 2002; Schindler, 2001]. Climate may significantly affect the flux of cations from catchments. Climate warming can enhance chemical weathering and the flux of basic cations from catchments to lakes [Sereda et al., 2011; Wright, Dillon, 2008] and can also intensify evaporation processes, which results in the concentration and salinization of aquatic systems. After prolonged droughts, which occur in southern regions in response to warming, the accumulation of salts in catchment becomes dangerous at the beginning of a rainy season, because salts can be rapidly transported into water reservoirs sharply increasing their salinity. When a lake is rapidly filled after a dry period, the

concentrations of cations will be lower than during their more steady supply from the catchment [Dillon et al., 1997]. In boreal regions, warming and increasing precipitation result in soil enrichment in water, and adsorption–desorption processes and organic matter decomposition in soils change, which results in the liberation and removal of basic cations (and possibly metals) into water streams. An increase in mean temperature, precipitation, and storm frequency observed in England and Scandinavia is related to climate variations in the past 15–25 yr [Bjerknes, 1964; Hurrell, 1995, Rodwell et al., 1999, Evans and Monteith, 2000]. The deposition of marine aerosols will stimulate salinization processes in catchments, and the intense transport of salts into terrestrial waters during rain periods following prolonged droughts may be a hazardous phenomenon.

It is obvious that production processes are enhanced in water bodies and catchments in warm climate, which may eventually result in eutrophication [Feuchtmayr et al., 2009]. On the other hand, warming-related processes in catchments enhance plant growth, uptake of nutrient elements, including nitrogen, and oxidation–reduction processes.

Much attention has been given to the influence of climate on wetland systems, with a special emphasis on the carbon cycle. Wetlands are widespread over the whole area of Russia and especially abundant in WS. On the one hand, they are peculiar traps of pollutants and stabilizers of the global carbon cycle, and they may become sources of secondary pollution under certain conditions, for example, during climate warming [Bayley et al., 1997; Dillon et al., 1997] showed that sulfate deposition over considerable wetland areas is accompanied by their reduction under anoxic wetland conditions. This is followed by the emission of sulfur-bearing gases, which are reoxidized in the atmosphere and transported over considerable distances. These processes are intensified during warmer periods.

A very hazardous phenomenon is the impact of warming on permafrost. Furthermore, the high degree of water logging in WS coupled with the tendency of precipitation increase owing to climate warming in humid zones, which was noted in [Moiseenko, Gashkina, 2010; Pavlov, Malkova, 2005], will become more significant in the future causing the enrichment of lake water in organic matter. Other effects related to the paludification of catchments (acidification of waters and an increase in CI and mobility of some toxic metals) will also be strengthened. The warming of frozen peatlands in northern WS may increase the emission of CH4 and other greenhouse gases into the atmosphere. The intensification of thermokarst processes will result in an increase in the number and area of lakes.

Thus, the results of investigations published in recent years highlighted the problem of the influence of climate variations on the development of water chemistry. However, controversial estimates were reported in the literature on the consequences of warming for terrestrial waters. The character of temperature influence is determined primarily from changes in the hydrologic conditions of water formation and biogeochemical cycles, i.e., the amount of precipitation, existence of a snow cover, state of bedrocks in the catchment, degree of their depletion in exchange bases, accumulation of P (or acid forming agents) in the catchment on the historical timescale, microbiological activity, and acceleration of plant growth.

The results of our studies of lake water chemistry in a latitudinal gradient (from tundra to arid zones) revealed general trends of changes in the chemical composition of water depending on temperature gradient; this provided a scientific basis for the theoretical prediction of possible changes in the hydrochemistry of lakes in response to a temperature increase. The chemical composition of water is controlled by a number of factors, which may enhance or suppress the geochemical processes of water formation. Let us consider the influence of climate variations via changes in the main mechanisms of the development of water chemistry on the basis of the results of our investigations.

Influence of temperature on the hydrochemistry of WS lakes. No special long term investigations of the influence of climate warming on the chemical composition of lake water were carried out in WS. Hydrochemical changes can be predicted only on the basis of correlations between the general characteristics of the chemical composition of lake water and temperature characteristics of the area. Such relations can be estimated on the basis of the extensive investigations of 2010–2012 on the hydrochemical parameters of WS lakes from tundra to steppe (Fig.1, 2 in the presentatons).

Factor and regression analysis demonstrated that the climate parameter, the sum of active temperatures ($\Sigma t > 10°C$), is closely related to the water salinity indicator

(Σ_{ions}), which increases in response to climate warming. A correction was introduced to account for the degree of paludification in the catchment (K_m), which strongly influences the chemistry of natural waters in WS. The following regression equation was derived:

$$\Sigma_{ions} = -6.98 + 13.55\exp(0.002\Sigma t > 10°C) - 2.69Km \quad (1)$$

It was found that this empirical equation is most useful for the middle taiga, southern taiga, and forest steppe. The influence of permafrost is significant in northern regions, and relations between landscape components are different; therefore, another relation was derived:

$$\Sigma_{ions} = 202.39 - 0.37\Sigma t > 10°C + (\Sigma t > 10°C)2\ 1.442K_{runof} - 0.31K_m \quad (2)$$

which includes corrections for both the degree of paludification, Km, and annual runoff, K_{runoff}. The increasing role of surface runoff in the formation of the total salinity of lake water can be explained by the fact that a higher fraction of water is transported from the catchment to the lake basin in the permafrost zone.

The prediction of changes in lake water salinity for the permafrost using Eq. (2) suggested that a temperature increase of 1.0°C may have different effects on salinity; in particular, a slight increase in salinity is observed in the tundra, and a slight decrease is characteristic of the northern taiga. This is related to the effects of two opposing phenomena. On the one hand, the thawing of salt-bearing rocks of marine origin, which are widespread in the Yamal and Gydan peninsulas, will enhance the chemical weathering and leaching of ions; an increase in precipitation will exert diluting effects in permafrost zones.

Calculations using Eqs. (1) and (2) showed that temperature changes of 1.0–10.0°C will not significantly increase the accumulation of ions in lake water in all of the natural zones. The salinity will even decrease in waterlogged taiga areas, because freshwater mono-mineralic (90% quartz) sand and sandy loam fluvial and alluvial deposits, which are common in the taiga zone, cannot supply significant amounts of ions even at intense chemical weathering. Therefore, further freshening of taiga lakes can be expected in response to climate warming and a corresponding increase in soil moisture content.

A temperature increase activates eutrophication owing to the enhancement of the removal of P, N, and dissolved organic matter in all zones except for tundra; however, no significant correlation was observed between the P content and the climate parameter.

An increase in moisture content in landscapes will result in the progressive development of wetland systems. The ubiquitous water logging of the taiga zone of WS is very important for the evolution of the chemical composition of surface and ground waters. Before penetrating into the saturation zone of an aquifer system, precipitation percolates through a peat layer and acquires unfavorable physicochemical properties (low content of dissolved oxygen, low salinity, high acidity, high organic matter content, and high oxygen demand). Correspondingly, all the aforementioned hydro-chemical characteristics will rise.

Water soluble salts and carbonates are especially abundant in the rocks of the northern Yamal Peninsula, the fraction of freshwater glacial and fluvial sediments increases southward and inland at the expense of salt-bearing marine deposits [Yamal Peninsula, 1975]. There is no significant increase in salinity with increasing temperature even in the forest steppe and steppe zones of WS, in contrast to ER, where the predicted increase is as high as 25% [Moiseenko and Gashkina, 2010].

Summarizing the analysis of landscape–hydrological and hydro-chemical transformations of the water of small lakes in response to climate changes, it should be noted that a temperature increase is the primary cause and the first member in the chain of rather significant changes in natural processes. An increase in air temperature will be followed, especially in spring and summer months, by a temperature increase in soils and rocks, an increase in the depth of seasonal thawing of soils in the catchments of lakes in the permafrost zone, and acceleration of erosion processes in humid areas. The tundra, forest tundra, and taiga zones will show an increase in the amount of precipitation, runoff to lakes, and the rate of biological cycling in plant communities and soils of lake catchments. In contrast, the forest steppe and semiarid zones will show an increase in the salinization of soils and lake waters, whereas a decrease in the amount of precipitation will reduce water runoff from catchments, but this process will be less evident compared with that predicted for the lake water of ER.

An important consequence of transformations in natural complexes owing to climate warming in the WS taiga will be a change in the hydrologic and biochemical balance of wetland ecosystems. An increase in the amount of precipitation will enhance paludification, which will result in enrichment in metal humates, a pH decrease owing to the release of free H+ from initially frozen peatlands, and general intensification of reducing processes. The reduction of Fe and Mn compounds in gleyed soils will further enrich lake waters in Fe-bearing organometallic compounds, which will result in an increase in already high CI.

The currently observed global and regional climate warming will affect in the future the biogeochemical cycles of the catchments of lakes and the total salinity and ionic compositions of waters will change accordingly. Dramatic changes in water salinity are not expected in humid zones owing to the mutually compensating effects of chemical weathering, thawing of frozen rocks, and dissolution of salts by the increasing amounts of precipitation and fresh soil waters and groundwaters. An increase in the seasonal variability of water salinity is predicted, especially for the semiarid and arid zones of WS. A temperature increase activates eutrophication processes owing to the more intense removal of P, N, and dissolved organic matter in all natural zones.

The influence of warm periods on the contents of nitrates, organic matter, and marine salts was noted. However, the available estimates of the consequences of a temperature increase for terrestrial waters are ambiguous. The character of temperature influence is primarily manifested through changes in the hydrologic conditions of water formation and biogeochemical cycles, i.e., the amount of precipitation, presence of a snow cover, state of bedrocks in the catchment, degree of soil depletion in exchange bases, accumulation of P (or acidforming substances) in catchment on historical timescales, microbiological activity, and enhancement of plant growth.

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Longterm variation of chemical elements fluxes from river basins in Central Siberian Plateau, underlain by permafrost

SCIENTIFIC ORGANIZATION

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ABSTRACT

Subarctic rivers in Central Siberian Plateau have specified fed-characteristics due to permafrost distribution and dynamics of active layer thawing. Two watersheds were studied – Nizhnyaya Tunguska and Tembenchi. Total flux of anions and cations from two watershed – Nizhnyaya Tunguska (1960-2011) and Tembenchi (1970-2011) – has been increased since 1960 to 2011 from 6, 38 to 32,72 Mg/km2/year and from 14,45 to 20,37 Mg/km2/year, respectively.

KEYWORDS

Permafrost, fluxes, watersheds, trace elements, Central Siberian Plateau, river basin, elements' export.

SUMMARY

Subarctic rivers in Central Siberian Plateau have specified fed-characteristics due to permafrost distribution and dynamics of active layer thawing. During the winter mean water period the greatest contribution in river feeding is made by ground water discharged through taliks, during the frost-free period – by precipitation, infiltrating in soil (Prokushkin et al 2011).

On the basis of climate data analysis, which indicates that temperature, precipitation and water discharge have been increasing during last 50 years for Central Siberian rivers, our objective was to estimate elements' fluxes from river watersheds, situated on Central Siberian Plateau – Nizhnyaya Tunguska and Tembenchi. This study could give an idea of tendency of biogeochemical processes' intensity on river basins, underlain by permafrost. We had for an object to calculate elements' fluxes (HCO3-, SO42-, Cl-, Ca2+, Mg2+) from the Nizhnyaya Tunguska river basin (for the period 1970-2011) and from the Tembenchi river basin (for the period

1960-2011). The first river basin has watershed area of 268000 km2 and underlain by different types of permafrost, the second river basin has an area of 21600 km2 and underlain only by continuous permafrost. We have observed biogeochemical composition in studied rivers since 2004, sampling station is located in Tura, Russia. In addition, archive data for water discharges and biogeochemical composition (1960-2011) were received from Roshydromet.

Considering that there are insufficient amount of measurements in archive data, the studied period was divided on following intervals: (for Nizhnyaya Tunguska river - 1960-1969, 1970-1979, 1980-1989, 1990-1999, 2000-2009, 2010-2011; for Tembenchi river – 1970-1979, 1980-1989, 1990-1993, 2008-2011). For calculating daily fluxes, we applied the following stages: 1) elements' concentrations were multiplied by water discharges for all available dates; 2) then, we analyzed fluxes (F) dependence on water discharges (Q) for each anion and cation and we found that this dependence could be described by the function $F = a \times Q^b$ most significantly (a and b – coefficients). Confidence levels (p) for a and b were obtained with using STATISTICA 10 and all coefficients for entire period and all anions had necessary reliability ($p \leq 0.05$, or $p \geq 95\%$).

Studied ions concentrations have inverse relationship on water discharges. During flood time river water is diluted by melted water and their mineralization is increased (Kadamtseva 2005). During winter period concentrations of studied ions are increased as far as active layer freezes through, and taliks with composition specified by evaporate and whinstone become the main input source for rivers. As a result, within low water level in winter, when water discharges have a minimum of all year, total mineralization is increased (Kadamtseva, 2005).

Annual ions' fluxes from the Nizhnyaya Tunguska watershed has been increased: bicarbonate from 2.92 to 12.77 Mg/km2/year, chloride from 0.95 to 11.07 Mg/km2/year, sulfate from 1.13 to 2.79 Mg/km2/year, calcium from 1.48 to Mg/km2/year, magnesium from 0.4 to 1.44 Mg/km2/year). Thus, total flux of the main ions have been risen more than 4.5 times from the Nizhnyaya Tunguska river basin. There are probable causes of this increasing: 1) increasing high latitude rivers' water discharges (Peterson et al, 2002); 2) permafrost degradation caused by climate warming (Frey and McClelland, 2009), which may lead to changes in river feeding. Trend of changing in elements' fluxes from the Tembenchi river basin is different from that for Nizhnyaya Tunguska. The flux growth (from 1970 to 2011) was observed for following ions: bicarbonate (from 6.96 to 11.63 Mg/km2/year), calcium (from 2.46 to 4.84 Mg/km2/year) and magnesium (from 0.57 to 0.94 Mg/km2/year). However, the sulfate flux has been decreased from 1.47 to 0.4 Mg/km2/year and chloride flux varied from 1.88 to 3.39 Mg/km2/year without any trend. Nevertheless, the total export of main ions from the Tembenchi watershed increased from 14.45 to 20.37 Mg/km2/year since 1970 to 2011.

Two different data sources were described previously and some differences in flux values were obtained. For example, sulfate flow from the Nizhnyaya Tunguska river basin from 2005 to 2011 changed within 1.82 – 2.32 Mg/km2/year according to our data, and within 2.36 – 5.43 Mg/km2/year according to ROSHYDROMET data. Also for Tembenchi sulfate flux had significant decrease from 1.54 Mg/km2/year (1993, ROSHYDROMET data) to 0.54 Mg/km2/year (2005, our data). Such fact may cause by some distinctions in sampling and water analysis.

Total flux of anions and cations from two watershed – Nizhnyaya Tunguska (1960-2011) and Tembenchi (1970-2011) – has been increased since 1960 to 2011 from 6, 38 to 32,72 Mg/km2/year and from 14,45 to 20,37 Mg/km2/year, respectively. Possibly, quantity characteristic between Nizhnyaya Tunguska and Tembenchi may be caused by differences in average annual temperatures and different types of permafrost distribution on studied watersheds. Nevertheless, the increasing of total element flux from watersheds for entire period were obtained and. Such phenomenon could be accounted to climate changing and probable permafrost degradation.

Koltermann Klaus Peter

Dr rer nat, Professor

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Natural Hazards, Arctic and climate change

SCIENTIFIC ORGANIZATION

Moscow State University

ABSTRACT

Under the Mega-grant programme the “Natural Risk Assessment Laboratory” NRAL at MSU from 2010 – 2014 has focused on identifying natural risks in Russia’s coastal zone, estimating their probability and assessing their impact on specific locations or areas. The discussion will also address the lessons learnt in the mega-grant programme P220 and provide an outlook.

KEYWORDS

Natural hazards, risk assessment, climate change projections, socio-economic impact, CMIP5 scenarios.

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The work is supported by the Government of Russian Federation (agreements #11. G34.31.007 and #14.37.00038 with Moscow State University).

SUMMARY

In NRAL we drew on expertise in Earth Sciences, Sociology, Economics. Except for seismic events we looked at past, present and future pattern of wind-fields, temperature, precipitation, snow and permafrost and their individual and compound statistics. Besides using long observational records, retrograde model runs helped to understand the specific probability. Using the individual characteristics, or signatures of such extreme events, model projections of climate change, based on CMIP5 results were used to describe local and regional developments. In a second step, socio-economic characteristics for several areas or regions have reviewed under these climate change scenarios to describe the impact on natural conditions, land and economic use and development. This together with regional risk assessments are being used to increase awareness of natural hazards, provide input in designing preparedness measures and response design.

Since 2014, NRAL, with new funding, has moved to the Arctic Environmental Laboratory AEL to use previous findings and results, both methodological, scientific and technical, to address the specific problems of the Russian Arctic, both ashore and at sea. The main issue being addressed is the general water cycle, and the changes in its components under temperature changes due to climate change. The implications for permafrost, vegetation, and land cover are considerable, in the end affecting all forms of human use of the high Arctic.

The presentation will focus on the main results, their implications on science, administrations and indicate priorities for future implementation, i.e. in land use, infrastructure planning and economic management.

Komarova Tatyana
Ph.D. student

Environmental assessment of soil greenhouse gases fluxes in forest – fallow succession at the Central Forest Reserve in European Russia

SCIENTIFIC ORGANIZATION

Russian State Agrarian University – Moscow Agricultural Academy named after K.A. Timiryazev

ABSTRACT

The problem of global climate change is one of the key modern environmental problems. One of the principal factors influencing the current level of the greenhouse fluxes are land-use changes, including the forest restoration in fallow lands. The studies have been conducted in representative 5 sites at different ages of fallows. During the fallow succession there is a significant reduction in CO_2 emissions from soil. The most intensive CO_2 flux were in the afternoon from 12:00 to 18:00. The absolute values of soil emissions of CH_4 and N_2O are higher for fallow meadow grassland.

KEYWORDS

Greenhouse gases emissions, soil respiration, land-use changes, fallow, organic carbon of soils, Orthopodzolic soil, spatial diversity, soil dynamics, forest – fallow succession.

ACKNOWLEDGEMENTS

The studies were conducted with the support of the grant of the Government of the Russian Federation 11.G34.31.0079. The authors is grateful Vasenev V.I., Povetkin V.A., Ivanov A.S., Mazirov I.M., Lakeev P., Romanova N., Miloserdova Ju.

SUMMARY

The problem of global climate change is one of the key modern environmental problems. It is generally accepted that greenhouse gases (CO_2, CH_4, N_2O) accumulation is the main factor of Global climate change. One of the principal factors influencing the current level of the greenhouse fluxes are land-use changes, including the forest restoration in fallow lands – widespread at the Central Region of Russia.

We conducted the comprehensive environmental studies of soil greenhouse fluxes in comparable sites with different stages of the forest-fallow successions in the southern part of the Central Forest Reserve with spruce domination in the mature forest - representative southern-taiga ecosystems.

The principal studies have been done in 5 representative sites at different ages of succession:

1. Fallow meadow grassland («0» - moment);

2. Forest-fallow stage of 10-15 years with young birch domination;

3. Forest-fallow stage of 20-30 years with birch domination and young spruce participation;

4. Birch-forest after fallow stage of 80-100 years with spruce participation;

5. Spruce-forest after fallow stage of 120-150 years with birch participation.

Seasonal and diurnal dinamics CO_2 fluxes measurements were carried out in situ using a mobile gas analyzer Li-820 with soil exposure chambers and parallel observation of air temperature, soil temperature and moisture. Also, every ten days the soil air has been sampled in the vials for further CO_2, CH_4 and N_2O flux measurements by the stationary gas chromatograph.

The dominant soil type is Orthopodzolic soil (by Russia Taxonomy, or Alfisols by Soil Taxonomy, or Albeluvisols by WRB, or Sandy-loam podzoluvisols by FAO). Within forest-fallow successions there are shown the litter gradual development, humus-accumulative horizon differentiation, soil acidity and bulk density increasing. At the same time there is enough obvious in the down part of past-arable horizon gradual restoration of the podzolic horizon.

The monitoring results shown the essential decreasing of soil CO_2 fluxes «in 2 times» in frame of successions. The maximum CO_2 fluxes have been fixed in July with optimal temperature / moisture ratio. In the medial of July the maximum CO_2 emission is observed in fallow grassland (34,1 g CO_2 / m^2 day), that is almost «in 2 – times» more than in spruce-forest after fallow stage of 120-150 years. It is important that soil CO_2 fluxes essentially increase with soil temperature rise (with up to R = 0,75) and drop soil moisture (with up to R = - 0,66).

During the day, the most intense soil CO_2 fluxes have been observed from case of 12:00 to 18:00. The maximum CO_2 flux has been recorded at 15:00 in the fallow grassland (23 g CO_2 / m^2 day). In the forest-fallow stage of 10-15 years the maximum soil CO_2 flux observed at 12 hours was (16 - 17 g CO_2 / m^2 day). There were not strong differences in soil CO_2 fluxes of these two investigated sites in the «night» time from 21:00 to 9:00. The essential daily dynamics must be taken into attention for assessment the seasonal fluxes of greenhouse gases and carbon balance.

The maximum CH4 flux has been fixed in the fallow grassland and forest-fallow stage of 10 - 15 years - in stark contrast to stable soil sink CH_4 in the spruce-forest after forest-fallow older than 120 years (final stage overgrowth fallow). In the fallow meadow grassland there are observed CH_4 emission in July and sink in June and August, with a maximum flux in late June. The level of N_2O fluxes usually does not exceed 0,2 mg N_2O /m^{2*}day with the maximum flux in mid-August and light sink in early June.

Kurths Juergen

Professor

Head of Research Domain Transdisciplinary Concepts & Methods

Prediction of extreme climate events

SCIENTIFIC ORGANIZATION

Potsdam Institute for Climate Impact Research, Institute of Applied Physics of the Russian Academy of Sciences

ABSTRACT

We use new concepts from complex systems science to study predictability of extreme climate events. We first analyse and predict most of extreme rainfall events in the Central Andes. Second, we construct a new prediction for the onset of Indian summer monsoon which clearly outperforms existing methods. Stolbova et al., Geophys. Res. Lett. 43, 068392 (2016).

KEYWORDS

Prediction; precursor; critical fluctuations; air temperature.

ACKNOWLEDGEMENTS

The study is supported by Government of Russian Federation (agreement #14. Z50.31.0033 with the Institute of Applied Physics of RAS).

SUMMARY

We use new concepts from complex systems science to study predictability of extreme climate events and sudden regime transitions.

First, we introduce the concept of complex network divergence derived from a nonlinear synchronization measure. We apply this technique to real-time satellite-derived rainfall data and predict more than 60% (90% during El Nino conditions) of extreme rainfall events in the Central Andes. In addition to the societal benefits of predicting such natural hazards, our study reveals the responsible mechanism for this phenomenon.

Second, we use the complex network approach to identify tipping elements of the Indian monsoon. Regarding the onset and withdrawal of the summer monsoon as abrupt transitions, we find critical conditions before these events happen and construct this way a new prediction approach which leads to clearly outperform existing prediction methods of both.

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- N. Boers, R. Donner, B. Bookhagen, and J. Kurths, Climate Dynamics 45, 619 (2015)V, Stolbova, E. Surovyatkina, B. Bookhagen, and J. Kurths, Geophysical Research Letters 43, 068392 (2016)

ADDITIONAL INFORMATION

Co-authors: N. Boers, B. Bookhagen, V. Stolbova, and E. Surovyatkina.

Lebedev Sergey

Doctor of Sciences

Leading research scientist

Integrated Use of Satellite Altimetry in the Investigation of the Meteorological, Hydrological, and Hydrodynamic Regime of the Caspian Sea

SCIENTIFIC ORGANIZATION

Geophysical Center of the Russian Academy of Sciences

ABSTRACT

Oscillations in the Caspian Sea level represent the result of mutually related hydro-meteorological processes, which proceed not only in the sea catchment area but also far beyond it. Therefore, sea level monitoring and long-term forecast of sea level changes represent an extremely important task. This publication is to show the results of the application of satellite altimetry methods to the investigation of seasonal and interannual variability of the sea level, wind speed, wave height and dynamic in the Caspian Sea and Kara-Bogaz-Gol Bay.

KEYWORDS

Caspian Sea, satellite altimetry, remote sensing, sea level, wind speed, wave height, dynamic.

ACKNOWLEDGEMENTS

This study was supported by a series of grants of the Russian Science Foundation (No 14-17-00555)

SUMMARY

Estimate Background Concentrations of Dissolved Petroleum Hydrocarbons in the Baltic Sea Based on Remote Sensing Data and Simulation

Abstract

Oscillations in the Caspian Sea level represent the result of mutually related hydro-meteorological processes, which proceed not only in the sea catchment area but also far beyond it. The change in the tendency of mean sea level variations that occurred in the mid 1970s, when a long-term level fall was replaced by a rapid and significant rise, represents an important indicator of the changes in the natural regime of the Caspian Sea. Therefore, sea level monitoring and long-term forecast of sea level changes represent an extremely important task. The aim of this publication is to show the results of the application of satellite altimetry methods to the investigation of seasonal and interannual variability of the sea level, wind speed, wave height and dynamic in different parts of the Caspian Sea and Kara-Bogaz-Gol Bay. The work is based on the 1992 - 2015 TOPEX/Poseidon and Jason-1/2 datasets.

Litasov Konstantin
Professor
Leading staff scientist

Material transport in the deep Earth's mantle

SCIENTIFIC ORGANIZATION

V.S. Sobolev Institute of Geology and Mineralogy, Siberian Branch Russian Academy of Sciences

ABSTRACT

I discuss compositions of melt in the upwelling mantle, which can drive material transport under hot spots originated from the transition zone or core-mantle boundary of the Earth. An important requirement for plume motion would be stress-induced melting and dissolution-precipitation of the fusible component at the front and rear of the plume, respectively. Carbonatite melt is a likely candidate, especially for transition zone. In contrast, hydrocarbon-bearing melt can be the best candidate for the liquid portion of a mantle plume arising from the core-mantle boundary.

KEYWORDS

Earth mantle, transition zone, melting, plume, carbonate, carbonatite, hydrocarbons.

SUMMARY

The models considering fast mantle upwelling without an addition of volatile-bearing components are failed due to very high melting temperatures of mantle silicates. Without melting the material transport will be hardly possible. Thus, considering mantle plumes one should add fusible component to the system. In most geodynamic models fusible component is involved indirectly, for example, just changing the viscosity. Almost nobody try to consider the real process of melt movement through presumably non-porous mantle matrix or try to understand the nature of melt, which assist material transport in the very deep mantle. Some mechanisms, such as melt percolation or hydraulic magma fracturing, are applicable for lithospheric depths and cannot be considered as a reliable mechanism for deeper mantle with high plasticity and low porocity. The most likely mechanism, which can operate in the deep mantle to assist plume or diapiric ascent is the stress-driven dissolution-precipitation, however, the possible fusible component of plume melt in the deep mantle is a matter of debates. Here, I discuss possible compositions of melt in the upwelling mantle, which can drive material transport under superplumes and hot spots originated from the transition zone of from the core-mantle boundary.

The most likely candidates for fusible chemicals in the mantle plumes are alkali-bearing species, C-O-H volatiles, and carbonates. An important requirement for plume motion would be stress-induced melting and dissolution-precipitation of the fusible component at the front and rear of the plume, respectively. For this process one would have a volatile-bearing melt with low solubility of silicates (ca. 5-10%, but not zero) at the temperature of mantle geotherm (or slightly higher). The possible candidates are alkali-bearing silicate melt, hydrous silicate melt, carbonatite melt, and hydrocarbon-bearing melt. Alkaline silicate melt and hydrous silicate melt cannot be considered, since a huge amount of silicate can be dissolved in these melts and the process of plume ascent will be easily terminated by progressive reactions with the surrounding silicate matrix. Carbonated or carbonatite melt is a likely candidate, especially for transition zone. Phase relations in the alkaline carbonatite systems indicate that major melting of subducted carbonates should occur at the transition zone depths. Taking into account the amount of subducted carbonated (1-2 wt.% CO_2) in the top 500 m of model slab we proposed a model for mobile carbonatite melt diapirs, generating from the slab in the transition zone, migrating upwards, modifying and oxidizing possibly reduced mantle section, precipitating diamonds, creating enriched source regions, and initiating volcanism at the surface. Dehydration of stagnant subducted slabs in the transition zone may accompany carbonatite diapir formation, however significant involvement of hydrous species into melting in the transition zone is difficult due to very high solubility of water in ringwoodite and wadsleyite, the major minerals in the transition zone.

It should be noticed that carbonate or carbonatite melt may not survive through the lower mantle due to reduction to diamond or other carbon-bearing species (carbide) if we assume redox state of the lower mantle close to the iron-wustite (IW) buffer. Thus, hydrocarbon-bearing or hydrous hydrocarbon-bearing melt might be the best candidate for the liquid portion of a mantle plume arising from the core-mantle boundary. There is limited amount of information about hydrocarbon

phase relations and reactions with silicates in the lower mantle due to an extremely difficult experimental setup. The data for melting of volatile-bearing peridotite in the system buffered by the IW buffer at 1-3 GPa indicated negligible solubility of silicates in coexisting CH_4-H_2O fluid. However, recent melting experiments on peridotite and eclogite systems with reduced C-O-H fluid at 3-16 GPa indicated significant solubility of silicates in the coexisting C-O-H fluid. The diamond or graphite traps contained abundant microinclusions of silicates after experiments. The composition of fluid was not measured in the experiments, whereas theoretical estimates indicate a mixture of H_2O with methane and possibly heavier hydrocarbons. Similar fluid/melt containing H_2O and hydrocarbons with a relatively low solubility of silicate components along the mantle geotherm can exist through the lower mantle and can be considered as the most reliable candidate for the fusible component of mantle plumes from CMB. In support of hydrocarbon-bearing melt/fluid in the deep mantle, we demonstrated recently that formation of a hydrocarbon mixture is highly probable under reducing conditions at the core-mantle boundary.

Markina Margarita
PhD student
Research scientist

25-years wind wave hindcast for the North Atlantic

SCIENTIFIC ORGANIZATION

P.P. Shirshov Institute of Oceanology RAS

ABSTRACT

25-yr hindcast of wind wave characteristics over the North Atlantic is performed using third generation spectral wave model WAVEWATCH III in conjunction with non-hydrostatic mesoscale numerical weather prediction system WRF (Weather Research and Forecasting). The period of the hindcast covers 1989 up to 2013. The area of integration cover the North Atlantic Ocean from 20 to 70N and from 85W to 15E. Output of the hindcast (1-hourly) consists of basic statistics of wind waves for sea, swell and significant wave height, including characteristics of extreme waves.

KEYWORDS

WAVEWATCH, WRF, hindcast, significant wave height, North Atlantic, wave climate.

ACKNOWLEDGEMENTS

The work was supported by the Russian Ministry of Education and Science under the contract 14.B25.31.0026.

SUMMARY

Long term high resolution wind wave hindcast over the North Atlantic from 20°N to 70°N for the period from 1989 to 2013 has been developed with the third generation spectral wave model WaveWatch III in conjunction with the non-hydrostatic mesoscale NWP system WRF (Weather Research and Forecasting). The results were verified against buoys and satellite altimetry data.

Analysis of interannual variability of significant wave height based on the hindcast reveals negative significant trend in the Northeast Atlantic (both for mean and extreme characteristics) and in the eastern subtropics.

In the present study, we focused on understanding of variability in the significant wave height in the terms of probability density distributions of this characteristic using 2-parametric Weibull distribution. It effectively describes statistical properties of waves and fits well with observed and modelled probability of occurrence of wind and waves in most areas.

Probability distributions of waves and surface wind are strongly dominated by the shape parameter of Weibull distribution in the tropics with the scale parameter playing the major role in the mid and subpolar latitudes. In the period from 1989 to 2013 trends in the shape parameter of Weibull distribution are positive in the Labrador Sea and the Central midlatitude North Atlantic, which implies decreasing occurrence of high waves in these regions and negative in the subtropics and in the subpolar latitudes, implying growing occurrence of high waves. This result is consistent with the pattern of changes in statistical characteristics of surface winds.

Moiseenko Tatiana

Professor

Head of the department of biogeochemistry and ecology

SCIENTIFIC ORGANIZATION

V.I. Vernadsky Institute of Geochemistry and Analytical Chemistry RAS

Water quality and ecosystem health assessment to define environmental management strategies: case study of Ob and Volga rivers

ABSTRACT

Sustainable development assumes a balance between economic, social and environmental priorities. The Volga and Ob are the large rivers of Russian, large-scale contamination river's basins are caused by its geographical position within the industry developed regions of European Russia and Western Siberia. A comprehensive assessment is presented of the ecotoxicological situation in the Volga and Ob river's basins from the viewpoint of ecosystem health. The dose–effect dependencies clearly show that total pollution of rivers must be decreased, first for toxic contaminants.

KEYWORDS

Toxic impacts, water quality, metal bioaccumulation, ecosystem health, environmental management strategies.

ACKNOWLEDGEMENTS

The work was supported by grant of Russian Governments (№ 11G34.31.0036).

SUMMARY

A comprehensive assessment is presented of the ecotoxicological situation in industry polluted parts of Volga and Ob river's basins from the viewpoint of ecosystem health. Concentrations of organic and inorganic toxic substances in water are reported. Basic clinical and postmortem signs of fish intoxication are described; changes in the cellular structure of their organs and tissues, as well as disturbances in hemogenesis, developing under the effect of toxic agents, are characterized. The comparative characteristics of several microelements (Ni, Cu, Sr, Al, Zn, Co, Mn, Pb, Cd, Hg, As) found in fish are presented. The main disturbances to fish caused by the accumulation of microelements in their organs and tissues are also considered. Based on dose–effect dependencies calculated with respect to the total concentration of toxic substances, standardized to MPC, and fish health criteria, cases that exceed the critical levels of pollutants are demonstrated for the investigated river sections. Our results show that water quality and living conditions for aquatic species in polluted parts of Volga and Ob rivers are unsatisfactory. Based on the prevalence of signs of intoxication in fish, we can conclude that the ecosystem health conditions are quite dramatic and give a clear signal of the need to decrease toxic pollution.

The main question for environmental management is the level to which pollution loading must be reduced to achieve reference conditions and to preserve ecosystem health. To answer this question, we solved to accomplish three tasks :

1. Determinate how hydro-chemical information on water quality can be interpreted in terms of a unified parameter, which could reflect the real impacts of the dose taking into account contaminant complexes (multi-pollution);
2. Assign criteria for ecosystem health that informatively reflect the impacts of pollution;
3. Determine critical levels of water pollution and required load reductions based on a dose–effect relationship.

An integrated impact dose. In rivers and reservoirs, aquatic organisms are exposed to a mixture of all toxicants. It is important to find a numerical parameter describing the total toxic impact on fish. The integrated impact dose of contaminants is determined by their number, concentration and toxic properties. The values of GC or MPC differ by country, in spite of the fact that experimental research techniques to establish the MPCs are universal. For example, in Russia, the MPC values for Cu, V, Mn and some other elements are underestimated, whereas the MPCs for Cd, As, Pb, and Al are overestimated. However, despite these criticisms of the system of MPC, we used data on the toxicological properties of each toxicant based on

the MPC adopted in Russia. We have defined the integrated impact dose by summing the excess of real concentration for each of metals with their MPC as follows:

$I_{tox-1} = å(C_i/MPC_{fishery.})$.

I_{tox} is the integrated toxicity index; C_i are concentrations registered in water; $MPC_{fishery}$ are MPC for toxic substances accepted in Russia for aquatic life. According to Russian rules of water protection, the water quality may be considered good if I_{tox} is no more than one ($0 < I_{tox-1} \leq 1$).

Criteria of ecosystem health are the key aspects in the system of estimating critical levels of water contamination and water resource management. Fish health as an indicator of ecosystem health can be determined using methods such as clinical and postmortem examination, and histological, hematological, or biochemical studies. Determination of the critical levels of water contamination requires numerical biological criteria, which also adequately reflect the effect of toxic substances in the water. The following biological parameters were used as criteria for fish and ecosystem health (the average weighted for individual river sections): i) the percentage of fish in which the second or third stages of diseases were diagnosed; ii) the Z-index defined above; iii) the percentage of fish with hemoglobin concentration below 90 g/l and the low levels of neutrophils in the blood, etc.

Dose–effect dependencies and critical levels. Basing on dose–effect dependencies (between numerical indices of fish health and the chemical parameters of water quality, in particular the total concentration of toxic substances in the water standardized to MPC), the critical levels of water contamination was determined. The dose–effect dependencies were plotted for the above biological parameters. The accumulation of toxic metals can also enhance (and, in certain cases, even directly cause) pathologies in fish. Therefore, the relationship between the accumulation of microelements in fish and pathological disturbances in the organs and tissues of fish in polluted the Volga and Ob river's basins was analyzed. The dose–effect dependencies clearly show that total pollution of the Volga River must be significantly decreased, by at least 5–7 times, first for toxic contaminants. The study of the morphofunctional state, histopathology, accumulation of heavy metals and reproductive performance peled (*Coregonus peled*) of Ob river basins in the northern part of Western Siberia revealed the influence of heavy metal concentrations in fish on its diseases.

These studies have confirmed the high information value of the ecotoxicological approach to the assessment of water quality and ecosystem health, as well as the necessity of establishing more reliable MPC values. Note that ecotoxicological studies were carried out for the Volga and Ob river's basin for the first time, and many important river sections or reservoir areas were not investigated. In this respect, our studies could be considered "screening analysis of the ecotoxicological situation," but at the same time, they substantiate the information content of methodological solutions and the necessity of the continuation of large-scale studies in this field in the future.

The priority to preserve the natural potential (clean water, biodiversity, valuable fish stocks) needs to develop new approaches and complex decisions for improving ecological policy on the industry development territory. Economic and social optimum should be based on the conception of ecological expenditures - determination of the existing and possible damages from pollution and degradation of ecosystems. The main principle for determining the latter is cost of landscapes' re-cultivation, artificial purification of waters and man-made reproduction of fish resources.

ADDITIONAL INFORMATION

Laboratory of water quality, stability of water ecosystems and ecotoxicology has been created in 2010 in Tyumen State University. Leading scientist - Doctor of Biological Sciences, professor, an associate member of the RAS Tatiana Ivanovna Moiseenko. Grant No. 11G34.31.0036 (2010-2012).

Myasoedov Alexander

PhD

Researcher, Head of SOLab Developers Group

Storm Ice Oil Wind Wave Watch System (SIOWS): Web GIS application for monitoring the Arctic

SCIENTIFIC ORGANIZATION

Russian State Hydrometeorological University

ABSTRACT

The Satellite Oceanography Laboratory (SOLab) has developed the Storm Ice Oil Wind Wave Watch System (SIOWS) to solve the main issues encountered with satellite data and to provide users with fast and flexible tool for search, synergetic analysis and extraction of satellite data, model results and new satellite products created using developed methods and approaches for the purpose of early warning of hazardous weather events in the Arctic.

KEYWORDS

Arctic, web GIS, remote sensing, monitoring, forecasting, satellite data, modeling, synergistic analysis, data archives, interactive visualization.

SUMMARY

Working with satellite data, has long been an issue for users which has often prevented from a wider use of these data because of Volume, Access, Format and Data Combination. The purpose of the Storm Ice Oil Wind Wave Watch System (SIOWS, http://arctic.solab.rshu.ru/) developed at Satellite Oceanography Laboratory (SOLab) is to solve the main issues encountered with satellite data and to provide users with a fast and flexible tool to select and extract data within massive archives that match exactly its needs or interest improving the efficiency of the monitoring system of geophysical conditions in the Arctic.

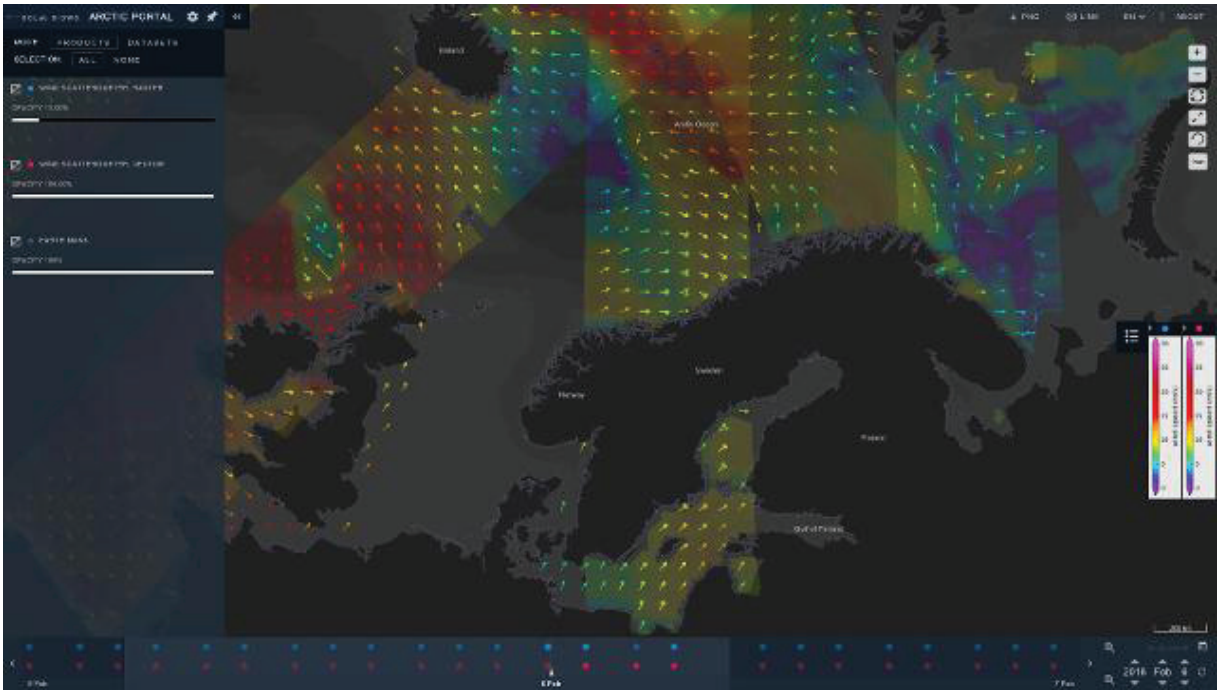


Fig. 1. Wind vectors from several ASCAT scatterometer datasets on 6 February 2016 displayed in SIOWS: Arctic Portal.

The following features will be implemented in the advanced SIOWS: Arctic portal (Fig. 1):

• implementation of the improved/new geophysical products developed in the Satellite Oceanography Laboratory,

• implementation of improved/new technologies of storage, processing and visualization of operational and archive data, including data overlay, their reprojection, visualization, animation and joint processing directly through a Web GIS SIOWS,

• implementation of the synergistic analysis of historical data,

• operational monitoring of the current state and dynamics of the system “ocean-atmosphere-cryosphere” in the Arctic region,

• forecast, based on the model of atmosphere dynamics WRF with assimilation of new satellite products - moisture content of the atmosphere, the sea-level pressure, wind, and sea surface temperature, and on the modifying resistance law, taking into account the features of the heat and momentum exchange on the border of the ocean-atmosphere system during high winds .

• prediction of anomalously high waves generation by moving atmospheric formation and their distribution in “real time” using the combination of the wind wave generation model and the WRF model

• identification of polar cyclones, vortex, oil spills, internal waves and swell waves

• use of created polar cyclones monitoring complex system for analysis of atmospheric, oceanic and ice conditions that determine origin and development of polar cyclones, and identifying patterns in their spatial distribution, intensity and frequency.

ADDITIONAL INFORMATION

Co-authors: Azarov S., Balashova E., Blokhin I., Grenishin A., Zabolotskikh E., Kudryavtsev V., Monzikova A.

Myslenkov Stanislav
Senior researcher

The frequency of storm events in the Barents Sea over the last 35 years

SCIENTIFIC ORGANIZATION

Lomonosov Moscow State University

ABSTRACT

The study of wave fields in the Barents sea was made by using WAVEWATCH III wave model. We get wind and ice cover fields data from reanalysis NCEP/CFSR (resolution 0.3°, time step 1 hour). We use special unstructured computing mesh which include the North Atlantic region from equator to pole with spatial resolution 1° and the Barents Sea with resolution around 0.3°. We made wave reanalisys from 1979-2015. The storm events where significant wave height higher then selected criterion (4, 5, 6, 7 m) was calculated. The distribution of storm events frequency is presented for each year.

KEYWORDS

Barents sea, wind waves, wave climate, wave modelling, WAVEWATCH III.

ACKNOWLEDGEMENTS

The work was supported by a grant RSF (project №14-37-00038).

SUMMARY

Introduction

Study of wave conditions in the Arctic seas of Russia is the priority task due to the oil and gas shelf fields development, maritime traffic over the North Sea Route and the related infrastructure development.

The mathematical modeling is the main instrument for wave studing because it is no sufficient observation data. Wave models can provide the data about wave parameters for the retrospective investigations and forecast information. The wind fields from the global reanalysis or forecast models are often use for this purposes [5, 7, 11, 12].

At the moment, the forecast of the wave in the Barents Sea is realized in the Hydrometeorological Centre of Russia by means of WW3 model [7]. The model has the space increment of 9 km and works on the GFS incoming data. The model quality check was carried out on the basis of the satellite data, and the results of the tests were obtained as satisfying.

Among the native works dedicated to the waves in the Barents Sea modeling, the work [12] can be singled out, where SWAN model was used for the shipping register drawing up, and the assessments showed good coincidence with the observation details.

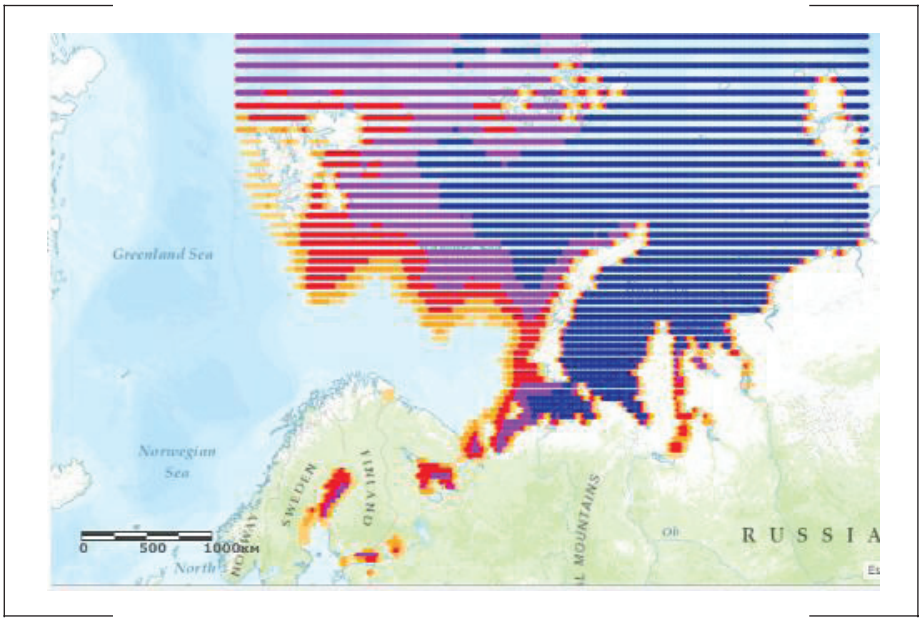
Computations and forecasts of the wind waving are also carried out with the usage of AANII (PD2-AARI) spectral and parametric model. The model was repeatedly verified by the data of the instrumental observations in the different waters and associated with such world famous models as WAM and WAVEWATCH. The results of the computations and forecasts accuracy statistical estimations are approximately similar for all models (mean root square error is around 0.5 m, the correlation ratio between the observed and calculated indexed is approximately equal to 0.9 [5, 11].

But it is no science investigations about temporal variability of storm events in the Barents Sea.

Data and methods

The study of wave fields in the Barents sea was made by using WAVEWATCH III wave model []. This model is very popular instrument for wave studying and it provide a good results []. We get wind and ice cover fields data from reanalysis NCEP/CFSR (resolution 0.3°, time step 1 hour). This reanalysis have a good spatial resolution and in work [] shown, that wind fields from this reanalysis have a good quality.

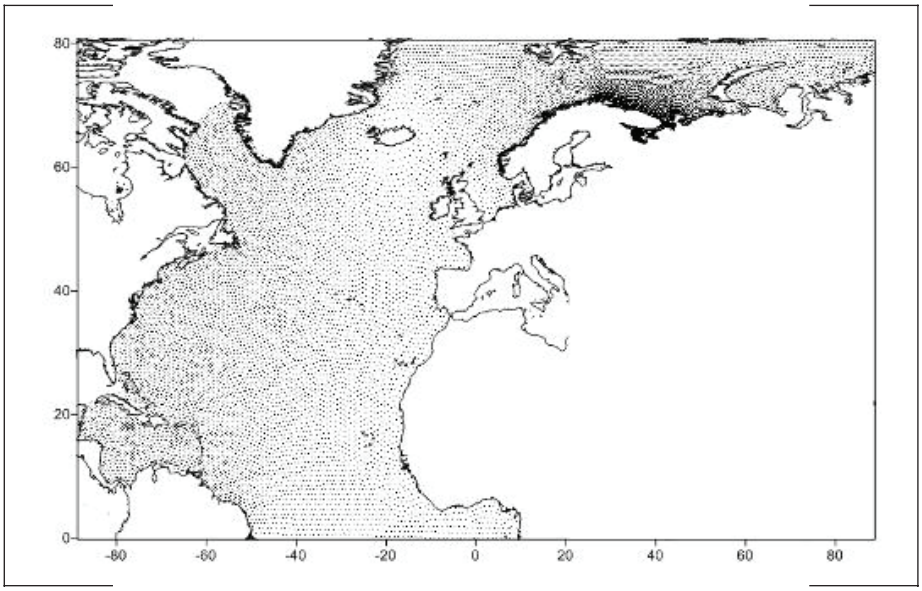
Fig.1. Example of the ice concentration in the Barents sea



The data about ice fields is very important for wave modelling in Arctic seas, because ice can seriously limit the wave growing and propagation (fig.1). We use special unstructured computing mesh which include the North Atlantic region from equator to pole with spatial resolution around 1° and the Barents with resolution around 0.2° (Fig.2). The main idea of using so big area in calculations was to minimize the open boundaries effects.

We made wave reanalisys from 1979-2015. The storm events where significant wave height higher then selected criterion (4, 5, 6, 7 m) was calculated. The distribution of storm events frequency is presented for each year.

Fig.2. The nodes of the computational grid for calculation wind wave in the Barents Sea



The implementation of spectral wave model SWAN for the Barents Sea, including the Northern part of the Atlantic Ocean was presented. Computations were performed by using special unstructured mesh, which has spatial resolution in the Atlantic Ocean is 1 °, in the Barents – 0.5 °. We already used this mesh in the previous studies [].

Preliminary results

Our wave data base for *the Atlantic ocean and the Barents sea includes the wave parameters (significant wave height, period, wave lengh, wave energy) with time step 3 hours. The example of wave field shows the spatial distributuon of significant wave height in the Atlantic ocean and the Barents sea (fig.3).*

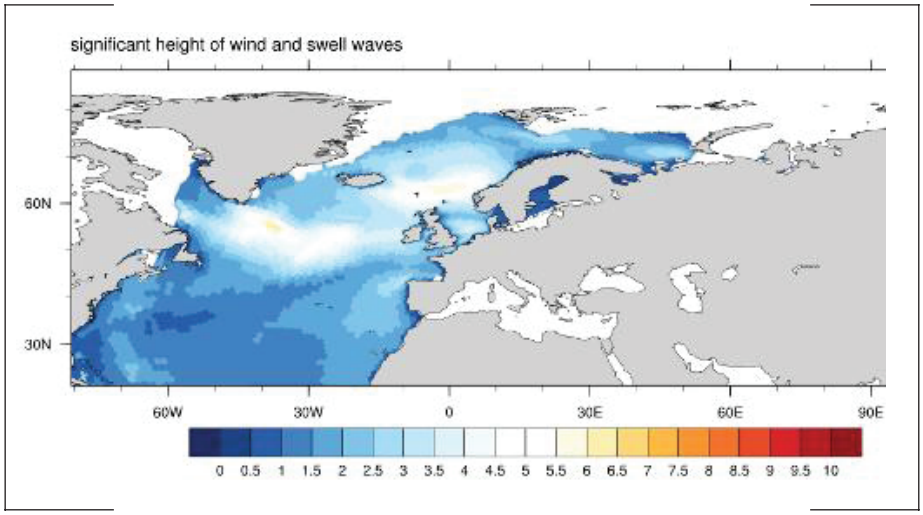


Fig.3. The field of significant wave height in the Atlantic ocean and the Barents sea

Than we calculated the storm events where significant wave height higher then 5 m (or enother selected height). It is a serius problem to separate the different events which suffices criteria only by machine algoritm and we used visual correction too. As a result we get the number of storm events for each year till 1979 to 2015. This allows to analyze the frequency of storms in different years.

Preliminary analysis shows that it is no strong trends in the frequency of storm events 1979-2015 but it was several periods when the storm activity was growing.

ADDITIONAL INFORMATION

Co-author: Markina Margarita.

Pokrovsky Oleg
PhD
Research Director

Biogeochemistry

SCIENTIFIC ORGANIZATION

French National Center for Scientific Research

ABSTRACT

Our center studies the climate-regulating role of Siberian wetlands via multidisciplinary approach that combines natural observations, laboratory experiments, and landscape-level modeling. The keywords of our research activity are carbon, green house gases, permafrost, peat, rivers and lakes. Although of mainly academic orientation, the applied component of our research will provide enormous social and economic benefits for the region and beyond.

KEYWORDS

Carbon, green house gases, permafrost, peat, rivers, lakes.

SUMMARY

The Environmental Context of western Siberia is extremely important for the biosphere and climate of our planet and highly attractive for Earth scientists for the following four reasons. In the **southern** part of western Siberia, the bogs are strong **CO_2 sink** from the atmosphere due to higly productive taiga forest and on-going peat formation

- In the **northern**, permafrost-bearing part of western Siberia, the bog-lake landscape system contain a lot of frozen organic carbon that is being **released to the atmosphere** in the form of methane and CO_2. Here, highly abundant thermokarst lakes act as important mediator of CO_2 from the frozen peat to the atmosphere.
- Western Siberia contains mostly discontinuous and sporadic permafrost, those temperature is between 0 and -2°C. Unlike usual continuous permafrost, this western siberian permafrost is **highly unstable, very vulnerable** to even the minor climate warming and can produce significaant environmental and economic effects within the next 1 – 2 decades
- Finally, the Ob river is dramatically different from the other Siberian and subarctic rivers because of its huge flood zone, the 2nd largest in the world after the Amazon Varzea. This **flood zone** represent so called **HOT SPOT in biogeochemical** cycles and essentially controls the flux of carbon and metals to the ocean from the full territory of western Siberia

These environmental factors and processes render western Siberia as **absolutely unique indicator** of on-going climate change, but it is also **strong regulator** of CO_2/CH_4 exchange with the atmosphere.

For this reason, we are taking **the advantage** of our unique geographical location, developed infrastructure and accumulated knowledge to characterize the **current status and future changes** of western Siberia low land mires.

What are the main advantages of our research center compared to our scientific groups working in boreal and subarctic region?

1. We investigate a **mega-profile over 2000** km latitude from south to north, located at otherwise similar lithological and orographic context but different climate, vegetataion and permafrost coverage
2. We always study **seasonal dynamics** of landscape parameters. To our knowledge, a few research groupss works on these issues in Siberia on year-round basis. To do state of the art research, one has to be located next to the study site.
3. We investigate rivers bogs and lakes and their full hydrological, biogeochemical and **landscape continuum** from the soil profile to the estuarine mixing zone
4. We use modern techniques which provide us a **multidisciplinary character**: including the expertise of trace metals and non-traditional isotopes; organic chemistry, microbiology, plant science, botany, physicis, limnology and hydrology
5. Two last but very important aspects of our work is that we combine the natural observations and filed work with **state-of-the-art laboratory experiments**
6. And, finally, we are among the few ones who already started large scale **biospheric natural manipulation** on selected water objects and bog zones.

Taken together, all this should provide un unprecedented level of prediction of future changes in the hydrosphere and landscapes, based primarily on ground observation combined with modeling and remote sensing techniques.

Repina Irina
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Modern Problems of Arctic research

SCIENTIFIC ORGANIZATION

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ABSTRACT

An expected consequence of the change to seasonal sea ice is a radical transformation of oceanic and atmospheric processes. This is a highly relevant and timely scientific topic of modern climate research. Addressing this challenge will help improve the reliability of long-term predictions as regards the environmental conditions, which is absolutely necessary for management and informational support of economic activities in the Arctic region, as well as timely adaptation/mitigation of social infrastructure and population livelihood to the rapidly changing climate.

KEYWORDS

Arctic Climate, ice cover, experivental research, climat models, remote sensing.

ACKNOWLEDGEMENTS

Grant of RSF 14-17-00647.

SUMMARY

The reasons for the accelerated changes in Arctic climate in recent years is still not clearly defined. The question remains about the relative contributions of internal oscillation and external influences (mostly anthropogenic) on the formation of climate change in the Arctic.

The most striking climate event of the recent two decades is the reduction of the summer Arctic sea ice area and extent. The absolute minimum of the sea ice extent for the entire period of satellite observations was reached in September 2012. Summer ice extent in 2005-2013 was also consistently lower than during the previous decade and substantially lower than the climate standard value. After a drastic decrease of the sea ice area in summer 2007, the ice cover over a substantial part of the Arctic Ocean became seasonal. According to the projections of the Global Climate Models (GCMs), totally seasonal Arctic Ocean ice cover is expected to emerge by the second half of the 21st century. However, accelerated summer melt/removal of ice from the deep Arctic Ocean interior in the last several years probably requires revision of this time frame. An expected consequence of the change to seasonal sea ice is a radical transformation of oceanic and atmospheric processes caused by fundamental change in the state of the ocean surface. This transformation may invoke/accelerate non-linear feedbacks in the "ocean-ice-atmosphere" system. Deep understanding and comprehensive investigation of the present changes in the Arctic climate system components is ultimately needed for adequate representation in the GCMs. This is a highly relevant and timely scientific topic of modern climate research. Addressing this challenge will help improve the reliability of long-term predictions as regards the environmental conditions, which is absolutely necessary for management and informational support of economic activities in the Arctic region, as well as timely adaptation/mitigation of social infrastructure and population livelihood to the rapidly changing climate.

The report focuses on the development of new methods of diagnosis and the simulation of the current state and evolution of the main components of the climate system in the Arctic (sea ice, permafrost, atmospheric boundary layer) in order to forecast its dynamics in a changing climate.

The influence of various factors on the current state of the ice conditions in the Arctic, as well as feedbacks between changes in the sea ice and regional atmospheric circulation is discussed. The estimation of the contribution of marine and terrestrial sources of greenhouse gases in the regional balance of atmospheric methane and carbon dioxide in the Arctic is proposed.

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Junior research scientist

ANN-based empirical model for ENSO forecast

SCIENTIFIC ORGANIZATION

Institute of Applied Physics of the Russian Academy of Sciences

ABSTRACT

The important task of modern science is construction of mathematical models of complex natural systems. There are two general approaches to natural systems modeling: (i) first-principle modeling, when mathematical model is based on physical laws, and (ii) empirical modeling, based on construction of model directly from data. This report is devoted to empirical modeling El-Nin'o (ENSO) from sea surface temperature anomalies data. We constructed model of evolution operator in form of artificial neural network and made forecast of the ENSO variability from several time points.

KEYWORDS

Natural systems, empirical modeling, evolution operator, ENSO, artificial neural networks.

ACKNOWLEDGEMENTS

The study is supported by Government of Russian Federation (agreement #14. Z50.31.0033 with the Institute of Applied Physics of RAS).

ADDITIONAL INFORMATION

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SCIENTIFIC ORGANIZATION

National Research Tomsk Polytechnic University, Pacific Oceanological Institute FEB RAS

Methane and carbon dioxide release from the East Siberian Arctic Shelf: The role of subsea and coastal permafrost and other controlling factors as inferred from decadal observational efforts

ABSTRACT

The East Siberian Arctic Shelf (ESAS) is employed as an integrator of ongoing changes in surrounding land, creating a terrestrial or exogenous signal which is carried by fresh water, and of in situ changes, creating a marine or endogenous signal, which is generated by submarine permafrost destabilization, increasing coastal erosion, and involvement of old carbon in the modern biogeochemical cycle. Misbalance in the regional carbon cycle causes severe ESAS water column oversaturation regards to atmosphere by the main greenhouse gases: methane (CH_4) and carbon dioxide (CO_2).

KEYWORDS

Arctic shelf, carbon, methane and carbon dioxide release, thawing permafrost.

ACKNOWLEDGEMENTS

The results of the project were achieved with support of the Government of Russian Federation/Ministry of Education and Science of the Russian Federation (contract number14.Z50.31.0012).We grateful our best colleagues from the International Siberian Shelf Studies/SWERUS-C3 Team & Tomsk Politechnic University, especially Ö. Gustafsson, A. Mazurov, S. Pugach, L. Anderson, M. Jakobsson, A. Charkin, J. Vonk, D. Chernikh, I. Leifer, D. Kosmach, T. Tesi, V. Tumskoy, L. Bröder, V. Samarkin, B. van Dongen, A. Salyuk and E. Panova.

SUMMARY

The Arctic region contains a huge amount of organic carbon (OC) buried inland and within the Arctic Ocean sedimentary basin, that is extremely sensitive to increased global temperatures because of the ice content of both on-land and submarine permafrost. The most pronounced warming is currently registered in the East Siberian part of the Arctic, where surface air temperature increased during the 2000-2005 period by about 5°C compared to 20th century temperature average. It is reasonable to expect that under conditions of continuing warming the regional carbon pool, which consists of OC in Siberian soil and sediments and seabed reservoirs of methane (CH_4), will be disturbed and signs of this disturbance will occur over the East Siberian Arctic shelf (ESAS).

The ESAS is employed as an integrator of ongoing changes in surrounding land, creating a terrestrial or exogenous signal which is carried by fresh water, and of *in situ changes*, creating a marine or endogenous signal, which is generated by submarine permafrost destabilization, increasing coastal erosion, and involvement of old carbon in the modern biogeochemical cycle. Eighty percent of all subsea permafrost underlies the ESAS. Increasing rates of coastal erosion and ongoing destabilization of both on-land and subsea permafrost have been altering the marine carbon cycle, and this could have a significant effect on global, not just Arctic, climate. Misbalance in the carbon cycle causes severe ESAS oversaturation regards to atmosphere by the main greenhouse gases: CH_4 and carbon dioxide (CO_2).

Sustained CH_4 release from thawing Arctic permafrost to atmosphere may be a positive, major feedback to climate warming. ESAS atmospheric CH_4 venting was reported as on par with flux from Arctic tundra *(Shakhova, Semiletov et al., Nature Geoscience, 7, 64-70, 2014, NGEO2007).* Unlike release when ancient carbon in thawed on-land permafrost is mobilized, ESAS CH_4 release is not determined by modern methanogenesis. Pre-formed CH_4 largely stems from seabed deposits. Our investigation, including observational studies using hydrological, biogeochemical, geophysical, geo-electrical, microbiological, and isotopic methods, and modeling efforts to assess current subsea permafrost state and the ESAS' contribution to the regional CH_4 budget, have clarified processes driving ESAS CH_4 emissions. Subsea permafrost state is a major emission determinant; rates vary by 3-5 orders of magnitude *(Shakhova, Semiletov et al., Phil. Trans. R. Soc. A, 373: 20140451).*

Progressive subsea permafrost thawing and decreasing ice extent could significantly increase ESAS CH4 emissions.

Subsea permafrost drilling results reveal modern recently submerged subsea permafrost degradation rates, contradicting previous hypotheses that thousands of years required to form escape paths for permafrost-preserved gas. Recently detected warmer water temperatures near the seabed may impact the stability of subsea permafrost and the carbon pool buried in the ESAS. As a result of these processes, subsea permafrost is degrading at higher rates than previously thought. Dissolved outer ESAS CH4 takes ≤1000 days to be oxidized because oxidation rates are low. Storms could release some aqueous CH4 to atmosphere; dissolved CH_4, captured beneath ice in winter, can spread via currents and escape to atmosphere through breaks in the ice.

We here use decadal data to show that extreme and extensive Ocean Acidification (OA) in the ESAS is caused not by direct uptake of atmospheric CO2 but rather by naturally-driven processes: carbon mobilization (and its oxidation to CO2) from thawing coastal permafrost/coastal ice complexes, and freshening due to growing Arctic river runoff and ice melt, which transport carbon along with freshwater to the ESAS *(Semiletov, Pipko et al., Nature Geoscience, 9,361–365, NGEO2695).* These processes compose a unique acidifying phenomenon that causes persistent, and potentially increasing, aragonite under-saturation of the entire water column. Extreme aragonite under-saturation in the western near-shore ESAS is associated with >80% depression of the total calcifying benthic biomass. Massive OA on the ESAS, the largest sea shelf system of the World Ocean, illustrates the complexity of the Earth system interacting with increasing anthropogenic pressure.

The significance of this research for world science is illustrated by publication > 40 papers in top journals, including *Biogeosciences, Geochimica et Cosmochimica Acta, Geophysical Research Letters, J. Geophysical Research, Marine Chemistry, Nature Communications, Nature Geoscience, Permafrost Pereglacial Processes*, and the opening remarks by Garry Nicholas-Roth, Editor in Chief of "G7 Climate Change: The New Economy" about Dr. Shakhova's *Foreword* (P. 16-17), which precedes transcripts of speeches by the G7 leaders: President Van Rompay (European Council), President Hollande (France), Chancellor Merkel (Germany), Prime Minister Abe (Japan), Prime Minister Cameron (United Kingdom) and President Obama (United States): *"This year's Foreword by Dr. Natalia Shakhova (key scientist in the project) is compelling and should be read with great trepidation and foresight"* /The G7 Summit, Brussel, Belgium, 4-5 June, 2014 (http://cloud.digipage.net/go/g7climatechange2014/).

ADDITIONAL INFORMATION

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Complex laboratory modeling of the transfer processes between atmosphere and ocean in the boundary layers

SCIENTIFIC ORGANIZATION

Institute of Applied Physics
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KEYWORDS

Atmosphere, ocean, laboratory modeling, turbulence, waves, wind.

ACKNOWLEDGEMENTS

The work was supported by the Russian Ministry of Education and Science (Contract No. 14.616.21.0059, unique identifier RFMEFI61615X0059).

SUMMARY

The main quantitative characteristics of atmosphere and ocean turbulent exchange are fluxes of momentum, heat and moisture. These fluxes play an important role

in many aspects of meteorological and oceanographic research, including climate modeling, weather forecasting, modeling of boundary-layer processes etc. Turbulent exchange of energy and momentum between the ocean surfaces and the atmosphere to a large extent controls the energy and water cycle and general circulation of the ocean and the atmosphere. The most important characteristics that determine the interaction between the atmosphere and the ocean are flows of momentum, heat and moisture. For their parameterization the dimensionless exchange coefficients (the surface drag coefficient *Cd* and the heat transfer coefficient or the Stanton number *Ch*) are used. The purpose of this study is the investigation of the effect of surface waves and foam on the turbulent exchange of momentum and heat within the laboratory experiment, when the wind and wave parameters are maintained and controlled. The effect of spray on turbulent exchange at stormy and hurricane winds is also estimated.

Laboratory modeling provides unique possibilities for investigations these processes for a wide range of wind and roughness parameters.

A series of experiments to study the processes of turbulent exchange of momentum and heat in a stably stratified temperature turbulent boundary layer air flow over the waved water surface was carried out at the High Speed Wind - Wave Stratified flume of IAP RAS (length 10 м, cross section of air channel 0.4 m by 0.4 m). The peculiarity of this experiment was the option to change the surface wave parameters regardless of the speed of the wind flow in the channel. For this purpose a polyethylene net (0.25 mm thick and a cell of 1.6 mm by1.6mm) has been stretched along the channel. The net does not affect the heat exchange, but the characteristics of surface waves depended on the position of the net: the waves were absent when the net was located at the level of the undisturbed water surface, and had maximum amplitude at the maximum depth of the net (33 cm). To create a stable temperature stratification of the wind, the air entering the flume was heated to 30-40 degrees. The temperature of the water surface was maintained constant about 15 degrees. The air flow velocity in the flume corresponded to the 10-m wind speed from 10 to 35 m/s. The turbulent fluxes of heat and momentum were retrieved from the velocity and temperature profiles measured with Pitot and hotfilm gauges at the distance 6.5 m from the inlet of the flume and subsequent data processing exploiting the self-similarity of the temperature and velocity profiles. As a result the surface drag and heat exchange coefficients as well as roughness parameters were obtained. Wind wave spectra and integral parameters (significant wave height, mean square slope) were retrieved from measurements by a 3-channel array wave gauge by coherent spectral data processing. To estimate the amount of spray in the air flow, as pray marker was introduced using the effect of a sharp decline in hot film readings in contact with a droplet.

The dependences of the exchange coefficients on the winds speed, the wave parameters and spray marker were obtained. It is shown that the exchange coefficients increase with the wind speed and wave height. It was found, that a sharp increase of the drag and heat exchange coefficients at wind speeds exceeding 25m/s was accompanied by the emergence and increasing concentration of the spray in the air flow over water. The correlation coefficient between the drag coefficient and the spray marker was about 0.75.

The effect of foam presence on the transfer processes and the parameters of the surface roughness within the laboratory simulation of wind-wave interaction was also studied, using a specially designed foam generator. The parameters of air flow profiles and waves elevation were measured with scanning Pitot gauge and wire wave gauges respectively in the range of equivalent wind speed U10 from 12 to 38 m/s (covering strong winds) on the clean water and with foam. It was shown that the foam reduces the amplitudes and slopes of the waves in comparison with the clean water in the hole range of wind speeds investigated, and the peak frequency and wave numbers remain almost constant. The drag coefficient calculating by profiling method demonstrated similar behavior (almost independent on U10 for the strong winds) for case of foam and increased compared with clear water, particularly noticeable for low wind speeds. Simultaneously the investigations of influence of the foam on the peculiarity of the microwave radio back scattering of X-diapason was investigated. These measurements were carried for different sensing angles (30, 40 50 degrees from vertical) and for four polarizations: co-polarized HH and VV, and de-polarized HV and VH. It was shown that foam leads to decrease of specific radar cross section of the wavy surface in comparison with clean water.

Overview of the High Speed Wind - Wave Stratified flume of IAP RAS of IAP RAS

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Linking successional development of soils in the Maritime Antarctic to belowground processes using a combined stable carbon isotope and metabolomics approach

SCIENTIFIC ORGANIZATION

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ABSTRACT

Changes during soil development are closely linked to vegetation succession and ecosystem functioning. The Maritime Antarctic provides an ideal setting to study this processes. Here, we present a first attempt to combine a stable isotope approach with soil metabolomics on a soil chronosequence to unravel the effects of plant succession on belowground soil processes. We show that the advent of the higher plant Deschampsia antarctica strongly impacts carbon allocation belowground with distinct consequences on soil microbial processes and soil CO2 efflux.

KEYWORDS

Carbon allocation, climate change, metabolomics, NLFA, PLFA, plant succession, pulse-labeling, stable isotopes, soil carbon, soil formation, soil CO_2 efflux.

ACKNOWLEDGEMENTS

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SUMMARY

Background

Research on ecosystem functioning under changing abiotic conditions have been under increasing attention of the scientific commnunity since decades. Maritime

Antarctica is among the sensitive areas, which are severely affected by climate change. Global warming in the Antarctic Peninsula with temperatures rise in about 0.06 $^{0}C\ y^{-1}$ within the past 45 years has accelerated rapid glacier retreatment forming temporal gradients of soil development region (Convey, 2003; Cook et al., 2005; Sancho et al., 2007). The changes in abiotic parameters reflected in ecosystem dynamics and functioning, and particularly, in vegetation succession are closely linked to soil formation.

Over the last three decades, significant and relatively rapid colonization of the ice-free soils by two vascular plant species (*Deschampsia Antarctica* and *Colobanthus quitensis*) has been recorded, indicating biological responses to rapid environmental change in this region (Gerighausen et al., 2003; Parnikoza et al., 2009). Coincidently, due to the fostered interaction to soils, plants are also able to modulate soil development and have a significant impact to ecosystem carbon balance at relatively short time scale.

In the past decade the paradigm emerged that above- and belowground processes are interconnected, e.g. plant photosynthesis is strongly linked with soil respiration. Recently gained carbon can be rapidly transferred belowground, fuelling the activity of microorganisms involved in decomposition of soil organic matter and mineral weathering, and influencing soil CO2 efflux rates on short-time scales (from hours to days) (Högberg and Read, 2006; Shibistova et al., 2012).

The features and different patterns of carbon allocation for numerous plants and ecosystems have been well documented, but such studies for Antarctic ecosystems, occurring in harsh conditions are lacking. Little is also known about the contribution of bacteria and fungi to decomposition of different soil carbon pools with different turnover rates in these soils, which is of utmost importance for the prediction of the future feedback of the Antarctic carbon balance to climate change. With this respect, it appears to be important to make a step in closing a gap in our knowledge on the impact of microbial and plant sources on soil organic matter composition of these soils.

Soil metabolomics is a powerful tool for comprehensive identification and quantification of all metabolites present in a biological sample (Coucheney et al., 2008), and is increasingly used to examine present interactions between organisms and the environmental conditions (Mashego et al., 2007; Coucheney et al., 2008), and to estimate the response of biological system to environmental modifications (Fiehn, 2002; Ossipov et al., 2014).

We were studying this on chronosequences, as they provide an ideal opportunity to study the impact of vegetation on the processes of soil formation. At Maritime Antarctica, glacier retreat chronosequences define sites that represent an increasing level of trophic complexity as a result of vegetation development. The goal of our study was to identify the *in vivo* biological activity and function in these soils along soil development. We approached this by following soil horizon formation, quantifying soil organic carbon stocks and carbon exchange with the atmosphere along a vegetation gradient at King George Island combining field CO_2 flux measurements, soil chemical analyses, ^{13}C in situ labeling and molecular methods (PLFA and metabolomics). Particularly, we aimed to compare the metabolic pools in the soils to reveal the impact of differences in the vegetation community composition and its possible link to the microbial population structure and activity.

Materials and Methods

We have chosen a rock outcrop (11-71 m asl) of the Collins glacier, representing a deglaciation chronosequence ranging from <200 yr B.P. to ~7200 yr B.P., with pronounced succession from algaea and cyanobacteria (i.e., bare soil) over lichens and mosses to the evolutionary younger vascular plant *Deschampsia antarctica*.

We applied a non-steady state chamber technique to measure carbon exchange between atmosphere and soil interphase. CO_2 fluxes were measured *in situ* using a portable infrared gas analyser (LI-COR 6400, Lincoln, NE, USA), coupled with a custom-made dynamic closed chamber within the vegetational gradient spanning bare soils, mosses, a mixture of mosses and *D. antarctica*, and pure *D. antarctica*. The GPP (Gross Primary Production) rates were evaluated from consequent measurements of net CO_2 exchange (NEE) with transparent and soil CO_2 efflux (SR) by opaque chambers, as following: GPP = NEE – SR and expressed in $\mu mol\ m^{-2}\ s^{-1}$.

A short-term *in situ* $^{13}CO_2$ pulse labeling of was carried out on February, 3, 2014 in Antarctica as described by Shibistova et al, (2012). The plant, soil and gas samples were collected daily within the chasing period. The soil $^{13}CO_2$ was collected by

NaOH absorption method followed by $SrCl_2$ precipitation. The stable carbon isotope composition was analyzed for leaves, roots, NLFA (neutral lipid fatty acids) and PLFA (phospholipid fatty acids), and soil- and plant derived CO_2 was determined by a an Elementar Isoprime 100 IRMS (Isoprime Ltd., Cheadle Hulme, UK) coupled to an Elementar vario MICRO cube EA C/N analyzer (Elementar Analysesysteme GmbH, Hanau, Germany).

We used the modified method of Gunina *et al.* (2014) to analyze PLFA in the soils collected in the field and stabilized in RNAlater® to prevent sample degradation (Schnecker et al., 2012). Lipids were extracted twice using a chloroform-methanol-citrate buffer (1:2:0.8 v/v/v), separated by solid phase extraction into glycolipids, neutral lipids, and phospholipids, hereafter analyzed by gas chromatography using an Agilent Technologies 7890A GC system equipped with a 60m Zebron capillary GC column (0.25mm diameter and 0.25µm film thickness; Phenomenex, Germany) and a flame ionization detector, using He as a carrier gas. Nonadecanoic acid (FA 19:0) was used as an internal standard. Seventeen PLFA were analyzed in total and the sum of all PLFA was used as a proxy of the microbial biomass and expressed as PLFA biomass. After conducting a principal components analysis (PCA) on data and relating the results to literature data (Zelles, 1999; Ruess and Chamberlain, 2010; Frostegård et al., 2011), we used the following markers to distinguish microbial groups: i15:0, a15:0, i16:0, i17:0, a17:0 and 18:1ω9c were used as markers for gram-positive bacteria (Gram+), 16:1ω5c, 18:1ω7c and Cy19:0 as markers for gram-negative bacteria (Gram–), 10Me16:0 to identify actinomycetes, 18:2ω6,9 as a fungal marker, 20:4ω6c to detect protozoa, and 14:0, 15:0, 16:1ω7c, 17:0, and18:0 as markers for unspecific bacteria.

The metabolites analysis was performed according to Ossipov et al. (2014). In brief, soils were collected in the field and stored frozen prior to analyses. In the laboratory, the samples were evaporated in the vacuum concentrator (Concentrator 5301, Eppendorf AG, Germany). After extraction and purification, followed by derivatisation, TMS derivatives of soil metabolites were transferred into an Perkin-Elmer autosampler vials with 0.15-mL glass inserts, closed by caps with septa, and analyzed with a Perkin-Elmer GC-MS system (GC Autosystem XL with TurboMass Gold quadrupole mass spectrometer, Norwalk, CT, USA). Mass spectrometer was used in the electron ionisation mode (EI^+) and ions were generated by a 70 eV electron beam. The data acquisition rate was set at 0.2 s, with a 0.1 s inter-scan delay and the recorded mass range 50 – 620 *m/z*. The column was a Perkin-Elmer capillary column (PE-5MS, 30 m, 0.25 mm i.d., film 0.25 µm) and helium was used as a carrier gas with a flow rate 1.0 mL/min. The injection volume of metabolite derivatives was 2.0 µL and the split ratio 20:1. The injector temperature was 290°C and the inlet line and the MS source were held at 300°C and 230°C, correspondingly. A series of *n*-alkanes (C_8-C_{20} and C_{10}-C_{40}, Fluka) were also analyzed to allow calculation of retention index (RI) (Kopka et al., 2005). Full scan output GC-MS files of all samples were converted into NetCDF format and an untargeted metabolomics approach was applied to process the data. MetAlign software (was used to extract and align all recorded masses.

Results and Discussions

Our study revealed that even under extreme environmental conditions, the appearance of higher plants was leading to the formation of well-developed soil, with high contents of organic carbon, with a relatively high rate of CO_2 soil efflux, and providing clear evidence of photosynthetic activity.

Along this chronosequence, there was a clear gradient of increasing formation of pedogenic minerals with increasing soil age. The development of a cryptic A horizon to well developed and increasingly thick O and A horizons at the older sites reflected organic matter accumulation from 0.2 kg m^{-2} at the bare soil to 3.6 kg m^{-2} under *D. antarctica*. An increasing photosynthetic activity from algae and cyanobacteria to *D. antarctica* was also mirrored by increasing soil CO_2 efflux rates along the chronosequence from 0.2 ± 0.1 to 2.8 ± 0.9 µmol m^{-2} s^{-1}. There was a strong temperature dependence of the soil respiration.

Isotope tracer techniques gave us the opportunity to follow carbon fluxes in the plant-soil system *in situ*. It has been found, that more than 15% of recently assimilated carbon was transferred belowground, of which approximately 2% of assimilated 13C was stored in roots within the chasing period. Carbon flow into soil fungi PLFA at adhering soil under *D. antarctica* was already recorded at the day 3 after labeling by a prominent ^{13}C peak, whereas ^{13}C excess in NLFA was steadily increasing during the chasing period. In contrast, bacterial PLFAs did not demon-

strate surficial tracer incorporation, despite of higher abundance of bacteria in rhizosphere. This suggests that rather not bacteria, but fungi preferentially and faster utilize the recently assimilated low molecular compounds allocated to the soil. This may bring a new insight to the dominating paradigm on distinct niching and specialization within decomposers society.

The metabolomics approach was applied to study the link between the successional stage of soils and its biological activity *in vivo*. Our soil metabolome database included 89 samples (observations) and 386 metabolites (variables). Application of multivariate statistics (SIMCA+) allowed selecting 57 metabolites as potential markers discriminating the soil horizons. Comparison of retention indexes (RIs) and mass spectra of the individual peaks with data from libraries allowed identifying of 86 metabolites (including some isomers). Among the identified low-molecular compounds carbohydrates, organic acids, alcohols and glycerides, lipophilic compounds (mainly alconoic acids) and sterols were detected. The identified carbohydrates were represented mainly by mono- (i.e., glucose, galactose, ribose and fructose) di- (i.e., maltose, melibiose, and trehalose) and trisacharides (raffinose and maltotrilose). Carboxylic acids (succinic, ethanedioic and azelaic) were found in all groups of samples.

The soil samples represent a complex mixture of metabolites with different chemical properties, concentrations and origin: plant and microbial derived compounds. The organic top-soils from both sites were characterized by high contents of metabolites, with prominent decrease of their relative abundances with soil depth. In most cases, the source of the metabolite could not be determined precisely as far as the most of the low molecular compounds are ubiquitous and inherently involved to metabolic cycles of plants and microorganisms. However, we identified some specific compounds, which could serve as specific biomarkers for different microbial groups. The soils sampled under vascular plant *Deschampsia antarctica* revealed the impact of the high plants on the soil organic matter, containing significantly higher amounts of carbohydrates and amines, as well as oleanolic acid - the basic oleanane-type triterpene, presumably as a result of root exudation.

We suggest, that metabolomics is a promising approach to assess the biological activity of soil in vivo and to distinguish of the contribution of plants and microorganisms to soil formation processes. Combined with other molecular studies (e.g. microbial biomarkers) and stable isotopes technique, it might been used as a powerful tool that yields additional information on the soil organic metter decomposition and thus the fate of assimilated carbon belowground.

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Arctic Research

ABSTRACT

The on-going development of the Arctic Region requires understanding of the possible limitations for the economic activity due to the specific of the Arctic environment. The absence of the experience often results in the unnecessary costs in maintaining the adaptation and mitigation measures in the region. Many threads to economic success are related to the Arctic-specific natural hazards. Analysis of their consequences has practical use in planning of the industrial development.

KEYWORDS

Arctic, Natural hazards, economic development.

ACKNOWLEDGEMENTS

The G.11.34.31.0007 project.

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SCIENTIFIC ORGANIZATION

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Paleoclimatology in Russia: recent progress and urgent needs

ABSTRACT

The talk will be focused on the technological achievements occurred in high resolution paleoclimatology in recent decades and on the gaps that should be filled out urgently due to disappearance (ice cores, tree-rings) or contamination (lake sediments) of paleoclimatic proxies that are deteriorating as result of human activity. Most promising paleoclimatic targets in Russia will be discussed.

KEYWORDS

Ice cores, climatic changes, high resolution reconstructions, glacier variations, tree-rings, lake sediments, tephrochronology, buried soils, climate models.

SUMMARY

Climate changes, their regional patterns, origin, and prediction are currently one of the most important scientific challenges. The functioning of the Earth climate system has a profound influence on the society development and human prosperity. The discrimination of human-induced and natural climate variability is one of the most urgent tasks and it cannot be solved using only the short instrumental meteorological observations and climate modeling experiments. Proxy records (tree rings, lake and marine sediments, ice cores, corals etc.) can be used to put into prospective to some extent the instrumental climatic records. Proxies can reach annual and seasonal resolution and they are useful for the large networks covering the areas of continental and even global scale. They can be calibrated against the instrumental data and this way they provide time series appropriate for the statistical analyses and numerical modeling. At this stage of developing of modern paleoclimatology it is essential to develop reliable regional reconstructions for the last millennia and before in order to increase our understanding of natural climatic variability.

Some of the most informative sources of paleoclimatic information are the ice core archives. However in the very near future many of them are in danger of completely vanishing due to the continued warming. Because of the increasing melting some mountain glaciers disappear. There are some glaciers in Russia where ice cores suitable for paleoclimatic analysis can be recovered. However, these unique archives are threatened by the warming, which in the coming years may delete the climatic signal due to the penetration of melt water into the interior of the glacier. Similarly in danger are other paleoclimatic archives of high resolution due to intense anthropogenic activity (old trees, lake sediments etc.). All of these unique paleoarchives in Russia also need to be rescued through being sampled, analyzed and organizing their proper long-term storage for the future generations. Comprehensive analysis of these paleoarchives will provide an opportunity to quantify variability of temperature (mean annual, summer), variability of precipitation (winter, summer). These reconstructions will allow performing validation of climate models for the last millennium. Thus they will provide a contribution to the solution of the global problem of change of the modern climate.

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Atmospheric buoyancy and tropical cyclones

SCIENTIFIC ORGANIZATION

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KEYWORDS

Atmosphere, buoyancy, tropical cyclones, potential energy.

SUMMARY

Buoyancy in the atmosphere connects net inward energy flux to emergent dynamic behavior. It is the trigger for convection occurring in local cells, but additionally aggregates into the hemispheric-scale flow patterns. Tropical cyclones form within and interact with this context. They do this both by actively consuming potential energy in the formation and intensification of their heat cycle, but they are addition-ally propagated by their contextual atmosphere flow, the Hadley and Walker circu-lations. Therefore the interaction between the two is of fundamental physical inter-est. To investigate this we use the state-of-the-art databases of tropical cyclone tracks and convection measures from the modern era reanalyses and analyse the connections on interannual and interdecadal time scales. For this purpose we use statistical approaches including EOF and SVD analysis.

Thiede Jörn

Prof. Dr. Dres. h.c.

Frontiers of Marine Geosciences, IODP The International Ocean Discovery Program: Will Russian marine geoscientists join the exploration of ocean floors through scientific drilling?

SCIENTIFIC ORGANIZATION

Saint Petersburg State University

ABSTRACT

Frontiers of Marine Geosciences, IODP The International Ocean Discovery Program: Will Russian marine geoscientists join the exploration of ocean floors through scientific drilling?

KEYWORDS

Ocean Drilling, Russian participation in IODP, Marine Geosciences, Earth System Science, Paleogeography of the oceans.

ACKNOWLEDGEMENTS

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SUMMARY

With 26 nations involved, the International Ocean Discovery Program (IODP) is worldwide the most prominent and forward looking marine research program addressing the planet Earth´s history and dynamics using ocean going research platforms.

IODP (Suyehiro 2015) builds on the legacy of the former ocean drilling programs which started with the Project Moho in 1961. The DSDP (Deep-Sea Drilling Project) has been using the drilling vessel GLOMAR Challenger from 1966 through 1984. In fall 1975 the IPOD (International Phase of Ocean Drilling) has started with Leg 45 and its expeditions covered almost the entire world ocean. IPOD comprised numerous international members including the Russian Acacdemy of Sciences, providing many participants to the IPOD expeditions (providing Russian participation both as regular scientists and as co-chief scientists who made very valuable and international recognized contributions to the results of DSDP). This evolved into the ODP (Ocean Drilling Program, 1985-2003) with the drilling vessel JOIDES Resolution. The IODP (Integrated Ocean Drilling Program) succeeded to ODP from 2003 to 2013 (without Russian membership). In addition to JOIDES Resolution, this program extended its research capabilities by introducing 1) a riser vessel provided by Japan, the Chikyu, to drill into geologically challenging locations, and 2) Mission Specific Platforms (MSPs) provided by ECORD (European Consortium for Ocean Research Drilling) to drill locations which cannot be investigated by the other platforms. Its successor, the International Ocean Discovery Program, began in October 2013 and has diversified the research themes linked to ocean drilling, in addition to reviving the original idea to drill through the Moho under the oceans.

The IODP expeditions function as „maritime universities" onboard of the drilling vessels providing opportunities of international cooperation and unique experiences, in particular to the young generation of marine geoscientists. In addition. ECORD offers a full array of high-profile educational activities for students and early-career scientists. We urge the Russian research authorities to persue an ECORD/ IODP membership, maybe through formation of a national consortium of interested institutions. Several levels of membership are possible and are open to negotations. Such a membership would provide opportunities to Russian scientists 1) to sail on the IODP expeditions, 2) to participate in its scientific planning/ advisory structure, 3) to submit new drilling proposals, and 4) to deploy sophisticated permanent monitoring devices embedded into new or existing drill holes. The perspective of potential future drilling in the Central Arctic (by ECORD in 2018) and in the Southern oceans would bring Russian marine geoscientists into regions of highest scientific interest.

Reference:
Suyehiro, K. 2015: Ocean Drilling.- Encyclopedia of Marine Geosciences, DOI 10.1007/978-94-007-6644-0_204-4, Springer Science+Business Media, Dordrecht.

ADDITIONAL INFORMATION

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New mechanism of sea-spray generation and heat-mass transfer under stormy conditions

SCIENTIFIC ORGANIZATION

IAR PAS

ABSTRACT

Basing on high-speed video we show that in air-flows with the surface stresses corresponding to the Force 8 wind, a special spray generation mechanism is activated. This regime is similar to bag-breakup mode of fragmentation of liquid in gaseous flows. Basing on general principles of statistical physics we develop statistics of the bag-breakup events, estimated the production rate of spray and showed, that at extreme winds "bag-breakup" is the dominant mechanism of sea spray production. This findings form a new basis for modeling the sea-spray and air-sea exchange at hurricane wind.

KEYWORDS

Sea spray, hurricane, polar low, heat-mass transfer.

ACKNOWLEDGEMENTS

This work was supported by the Russian Foundation of Basic Research (14-05-91767, 13-05-12093, 16-05-00839, 14-05-91767, 16-55-52025, 15-35-20953) and experiment and equipment was supported by Russian Science Foundation (Agreements 14-17-00667 and 15-17-20009 respectively), Yu.Troitskaya, A.Kandaurov and D.Sergeev were partially supported by FP7 Collaborative Project No. 612610.

SUMMARY

• Statistical analyses of sequences of frames of high-speed video has enabled us to prove that the dominant spray-generation mechanism in extreme winds relates to the bag-breakup fluid fragmentation regime. It activates at conditions corresponding to Force 8 wind, manifested as "spindrift".

• Starting from general principles of statistical physics, we develop statistics of the

bag-breakup events and determine the spray generation function, which is in good agreement with available experimental data.

• Large droplets generated by bag-breakup significantly contribute to enthalpy and momentum flux:

- They significantly increase the air-sea enthalpy flux at hurricane wind

- They enables to explain non-monotonous dependence of surface drag coefficient on wind speed peaking at 35-40 m/s.

The effect is more pronounced for polar low, than for tropical cyclones.

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Personal learning environment for competence in economic and societal impacts of local weather, air quality and climate

SCIENTIFIC ORGANIZATION

National Research Lobachevsky State University of Nizhni Novgorod

ABSTRACT

Nowadays people and organisations are ever more vulnerable to environmental factors. However, decision-makers at all levels often lack knowledge to account for economic and societal impacts of local weather, air quality and climate. The consequent damage and lost profit due to a non-optimal management decisions are already large and, if ignored, will inevitably become systematic. A new personal learning environment (PLE) is developed to change the situation.

KEYWORDS

Air quality, Economic meteorology, Environmental education, Internet of Things, Local weather, Microclimate, Personal learning environment, Urbanization, Wireless sensor networks.

ACKNOWLEDGEMENTS

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SUMMARY

Rapidly growing urbanisation, deterioration of environment, and climate change make people and organisations ever more vulnerable to environmental factors. Since 2009, the world has become more urban than rural: the number of people living in urban areas had surpassed the number of rural dwellers. Urban agglomerations, rapidly growing in size and number, form artificial environments with nature and properties poorly comprehended by the society.

With increasing complexity and heterogeneity of urban infrastructure, the modern life and economy progressively depend on local weather, air/water/soil quality, and microclimate. These comprise “personal environments”, controlled by physical and chemical processes in the lower atmospheric planetary boundary layer, directly interacting with the Earth’s surface and affected by industrial emissions and anthropogenic warming.

However, managers in weather-sensitive economic sectors, not to mention wide public, often do not possess sufficient knowledge about local environment and its impacts on their activities. The consequent damage and lost profit due to a non-optimal management decisions are already large and, if ignored, will inevitably become systematic.

The problem is addressed through development of personal learning environment (PLE) for enhancing competence in economic and societal impacts of local weather, air quality and climate. The PLE features custom-tailored learning materials, “smart” weather observation instruments, and learning management software – all integrated into a single system. Such approach allows for learning in contact with a studied physical environment and develops competences required for today’s modern life.

At first hand, the PLE is for university students of hydrometerology and economics profiles, hydrometeorology professionals, and managers at weather-sensitive firms and public bodies. Prospectively, it might prove useful to a wide range of customers, including secondary schools and private individuals.

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Mesocyclone activity over the Southern Ocean from satellite infrared mosaics for winter 2004

SCIENTIFIC ORGANIZATION

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ABSTRACT

Mesoscale activity over ocean surface plays a significant role in air-sea interaction and ocean heat loss process. To clarify the mesocyclone activity in Southern ocean and to produce reference database we manually tracked all mesocyclones in SO during winter 2004. In this study we used satellite infrared imageries by AMRC, and record location, diameter, cloud form and Synoptics of each cyclone. Using QuikSCAT scatterometer data we estimated uncertainty in cyclones wind characteristics reproducing in last generation of reanalyses. Number of polar lows was assessed.

KEYWORDS

Mesocyclones, polar lows, Antarctica.

ACKNOWLEDGEMENTS

This results are from collaborative project with scientific groups of professor Ian Renfrew (UEA) and Mathew Lazarra (University of Wisconsin).

SUMMARY

Number of studies demonstrates overview of mesocyclone activity over the Southern Hemisphere. These studies are based both on automated tracking algorithms and on manual identification and tracking and show inconsistent assessments. Due to high time consumption manual tracking studies are commonly regional.

To clarify the Southern Hemisphere mesoscale cyclone activity and to provide a reference dataset that may be used to validate automated tracking schemes in SH we manually tracked all mesocyclones over Southern ocean for winter of 2004.

In our study we used hemispherical infrared mosaics from Antarctic Meteorological Research Center, which covers polar region inside 40th degree with 3-hourly temporal and 5-km spatial resolution. At each time step we visually analyzed position of all centers of mesocyclones according to their cloudiness imprints in IR images, together with their radius according to Julie Harold, cloud form according to the classification of Andrew Carleton and large scale synoptics. We totally tracked 1735 mesocyclones during 500 hours of manual tracking.

Comma clouds occur more frequently than any other type of cloud forms. They typically occur in troughs of synoptic scale cyclones as surrounding. The ratio between comma and spiral clouds is 1:11, which is consistent with assessments of Cartleton, 1990. In terms of the spatial distribution of cyclogenesis, cyclolis and track density of cyclones we observe maximum mesoscale cyclogenesis and track density over Drake Passage and northward of Ross sea.

We found that mean diameter of mesocyclone in our dataset is 301 km, while other studies report from 300 to 1000.

Mean lifetime of our cyclones is 12 hours, they maximally live more than 2 days: they migrate to distances up to 2000 with mean 15 m/s propagation velocity. These characteristics of mesocyclones' lifecycle may be used in the future for effective threshold choice in automated tracking schemes. Next we validated reanalysis over the Southern hemisphere in reproducing wind speed characteristics in mesoscale cyclones against QuikSCAT Seawinds scatterometer. We evaluated maximum wind speed in cyclone (in R+50 km zone around its and center) and its location relative to the southern direction.

Maximum wind speed locates in cyclones mainly on periphery of vortex not only in scatterometer, but in reanalysis data too, what means that reanalyses reproduce cyclonic circulations, however the absolute values of wind speed are underestimated. The closest agreement with scatterometer data demonstrates MERRA2 reanalysis. Underestimation of maximum wind speed reaches 10 m/s for ERA Interim and JRA 55, and 5 m/s for NCEP CFSR and MERRA 2. Mean wind speed over the

cyclone area is underestimated from 1 to 5 m/s in NCEP CFSR and MERRA2 and Interim and JRA55 reanalysis accordingly. Using widely accepted threshold of 15 m/s we evaluated number of mesocyclones which belongs to polar lows class.

We revealed that the 15 m/s wind speed marks 85 percentile of wind speed in Southern Hemisphere, while maximum in the cyclone area wind speed 15 m/s corresponds to 50 percentile of empirical distribution. In this sense polar lows are mostly located over the Bellingshausen sea, Drake Passage and southern part of Indian ocean. They mainly occur westward of Drake Passage and than decay on Tierra del Fuego. The second storm track lies in southern Indian Ocean sector where cyclones are moving eastwardly.

72% of all our mesocyclone tracks fall into the polar low class, what is consistent with other study. In these areas they form from 40 to 100 % of total meosocyclone population.

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Integrated modeling

SCIENTIFIC ORGANIZATION

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ABSTRACT

Systems analysis and spatio-temporal modeling have been long recognized as powerful tools for decision support. However, the modeling results may go contrary to our preferences, biases and priorities making it difficult to act based on models. Integrated modeling has been successfully bringing together knowledge from various disciplines and making use of legacy models and code that have been previously produced. We see a lot of potential in taking model integration beyond software coupling, and in addition to computer models consider mental models developed by stakeholders.

KEYWORDS

Integrated modeling, participatory modeling, stakeholders, mental models, biases, interfaces.

ACKNOWLEDGEMENTS

Work was in part supported by the EU-FP7-308601 COMPLEX project.

SUMMARY

Systems analysis and spatio-temporal modeling have been long recognized as powerful tools for decision support. One of the biggest challenges is the need to synchronize our understanding of systems gained from models with human perceptions, beliefs, values and preconceived notions about the system. The modeling results may go contrary to our preferences and priorities. We find it then difficult to act based on the models and the logic of the system 2 type of thinking involved, when it clashes with the intuitive system 1 thinking. Integrated modeling has been successfully developing as a way to bring together knowledge from various disciplines and to use legacy models and code that have been previously produced. We see a lot of potential in taking model integration beyond the software coupling, and in addition to computer models consider mental models developed by stakeholders. Model integration should then deal with coupling of all sorts of models, including software components and conceptual models produced by stakeholders. Engaging stakeholders in the modeling process in a participatory process can help resolve some of these contradictions, though in many cases it is still difficult to organize and conduct the process properly. New technologies inspired by social media and wide access to the Internet deliver opportunities for broad democratic engagement of the public in science and decision making. However the process is easily compromised by increasing uncertainties associated with information production and sharing, group thinking, and clustering along cultural, educational or party lines.

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First climate smart agriculture approaches from results of RusFluxNet monitoring

SCIENTIFIC ORGANIZATION

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ABSTRACT

Potential increase in Russia's cultivated land, climate change and greenhouse gas emissions quotas make climate smart agriculture, as relevant as never before. Carbon budget was calculated at the fields in Moscow, for two agroecosystems with different crops from the same crop rotation studied for 2 years. Values about 200-250 g C m^2 per year may be considered as estimated values for the total carbon loss for agroecosystems with grain crops and grass mixt on sod-podzolic soils. The use of mustard as a green manure may reduce this value by three-quarters.

KEYWORDS

Eddy covariance, carbon budget, green house gases. climate smart, agriculture.

ACKNOWLEDGEMENTS

The study was performed under the support of RF Government grant № 11.G34.31.0079.

SUMMARY

Climate-smart agriculture is an complex approach to solve problems of food shortage and climate change, that definitely should address reducing greenhouse gas emissions from agriculture. Current political and economical situation in Russia with high interest and support to homeland food production can lead to spontaneous growth of agricultural land use.

At the same time, world facing climate change issues, which can lead to further development of quotas for greenhouse gas emissions. Several studies had shown that temperature increase in autumn-spring period leads to an increase in CO_2 emissions. For example, for Finland's forest with rather similar to Russian climatic conditions (T. Vesala et. al. 2010) carbon loss due to temperature change was estimated as 9 gC m^{-2} °C $^{-1}$. On other hand article of Stolbovoy, 2002, shown that loss of carbon from agricultural ecosystems in Russia, 9 times higher than from forest one's.

Therefore, potential increase in Russia's cultivated land, increase in temperatures in autumn-spring period and potential introduction of greenhouse gas emissions quotas make the issue of transition climate smart agriculture, as relevant as never before.

Carbon balance was calculated at the Precision Farming Experimental Fields of the Russian Timiryazev State Agricultural University, Moscow, Russia, for two agroecosystems with different crops from the same crop rotation studied for 2 years. The experimental site has a temperate and continental climate and situated in south taiga zone with Arable Sod-Podzoluvisols (Albeluvisols Umbric). The study was performed under the support of RF Government grant № 11.G34.31.0079

Meteorological and environmental conditions were similar for two towers (A and B) located on two adjacent fields, as expected. Also there were significant different in condition between years. Correlation coefficients between different years and different sites in microclimate measurements data were 0.83-0.99. Climatic features and crop type and phase were main drivers of NEE dynamics. Since both sites were placed on the same soil and climatic conditions were the same there were significant difference in ecosystem's respiration dynamics (Reco). But there were significant differences between sites in gross plant production due to differences in crops phenology (GPP).

Vertical fluxes of carbon dioxide were measured with eddy covariance technique, statistical method to measure and calculate turbulent fluxes within atmospheric boundary layers. Crop rotation included potato, winter wheat, barley and vetch and oat mix. Two fields of the same crop rotation were studied in 2013-2014. One of the fields (A) was used in 2013 for barley planting (Hordeum vulgare L.). The field B was

in 2013 used for planting together vetch (Vicia sativa L.) and oats (Avena sativa L.). Inversely oats and vetch grass mixt was sown in 2014 on field A. Winter wheat was sown on field A in the very beginning of September. On the second field (B) in 2014 winter wheat occurred from under the snow in the phase of tillering, after harvesting it in mid of July, white mustard (Sinapis alba) was sown for green manure.

Carbon uptake (NEE negative values) was registered only for the field with winter wheat and white mustard; because the two crops were cultivated on the field within one growing season. Great difference in 82 g C m^{-2} per year in NEE between two fields with vetch and oat was related to higher difference in yields. NEE for barley field was positive during the whole year; considering only the growing season, NEE for barley was 100 g C m^{-2} lower and was negative.

Closed balance for whole years showed that carbon losses were observed for all studied agroecosystems. It was minimal for field with winter wheat, with mustard, used as green manure, and it was maximal for field with vetch and oat mix.

Values about 200-250 g C m^2 per year may be considered as estimated values for the total carbon loss for agroecosystems with grain crops and grass mixt on sod-podzolic soils. The use of mustard as a green manure may reduce this value by three-quarters.

ADDITIONAL INFORMATION

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Hazardous hydrological phenomena and social vulnerability in Russia

SCIENTIFIC ORGANIZATION

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ABSTRACT

The purpose of the report is to estimate the influence of hazardous hydrological phenomena on society. Methods and results of social vulnerability and risk assessment are presented in the article. The field research was conducted in the Slavyansk municipal district in the Krasnodar region. The main result of the work is that social risk can be underestimated in comparison with economic risk because of a low “value of life” in Russia (no life insurance, neglecting of basic safety rules, etc.).

KEYWORDS

Socio-economic risks, economic damage analysis, social vulnerability index, hydrological hazards, risk assessment.

ACKNOWLEDGEMENTS

Koltermann Klaus Peter, Dobrolyubov Sergey Anatol’evich, Baburin Vyacheslav Leonidovich.

SUMMARY

Risk assessment is one of the most pressing scientific topics in Russia, but most of the works are devoted to natural hazards assessment. The purpose of the report is to estimate the influence of hazardous hydrological phenomena on society.

On the first stage, methods and results of social vulnerability and risk assessment are presented in the article. It is explored if modified methodology of the United Nations University (World risk index) can be used on different scale levels: regional, municipal and settlement. It was estimated that, despite the low value of the World risk index for Russia, southern coastal and mountain regions have high values of the risk index for hydrological phenomena because of higher frequency of the hazardous events, higher population density, and high social vulnerability. The Krasnodar region (in the south-western part of Russia) was chosen for a detailed analysis. A municipal risk index was developed, and municipal districts in the Kuban river mouth were identified as territories with the highest risk.

For verification of the index results, the percentage of vulnerable people was estimated based on opinion pollson the second stage. The field research was conducted in the Slavyansk municipal district in the Krasnodar region (the south-western part of Russia), which is a highly populated coastal territory with a high frequency of hazardous hydrological events.

Modified methods of the Ministry of the Russian Federation for Affairs for Civil Defence, Emergencies and Elimination of Consequences of Natural Disasters (EMERCOM) were used for potential economic damage calculation. The paper did not only focus on direct, tangible risks, but also included social risk (i.e. risk to life and health). Social vulnerability has been calculated directly as a percentage of vulnerable people, estimated in opinion polls, while in many recent papers the social vulnerability index was calculated as a combination of several statistical indicators. The resulting percentage of vulnerable people was converted to numbers of potential victims. Finally the social risk was expressed by financial indicators in terms of the cost of the value of statistical life lost.

The main result of the work is that social risk can be underestimated in comparison with economic risk because of a low “value of life” in Russia (no life insurance, neglecting of basic safety rules, etc.).

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Cognitive chaos: turbulence in Earth system

SCIENTIFIC ORGANIZATION

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ABSTRACT

Turbulence plays vitally important role in nature. In particular, it links geospheres via strongly turbulent boundary layers and performs vertical transport of energy, matter and momentum across atmosphere and hydrosphere. It never collapses even in very stable stratification and never dominates even in extremely strong convection. This happens due to tricky self-control mechanisms keeping chaos and order in the atmosphere and hydrosphere in the shares optimal for the Earth system.

KEYWORDS

Atmosphere Boundary layers, Chaos, Convection, Earth system, Hydrosphere, Order, Turbulence, Stratification, Self-control, Vertical transport.

ACKNOWLEDGEMENTS

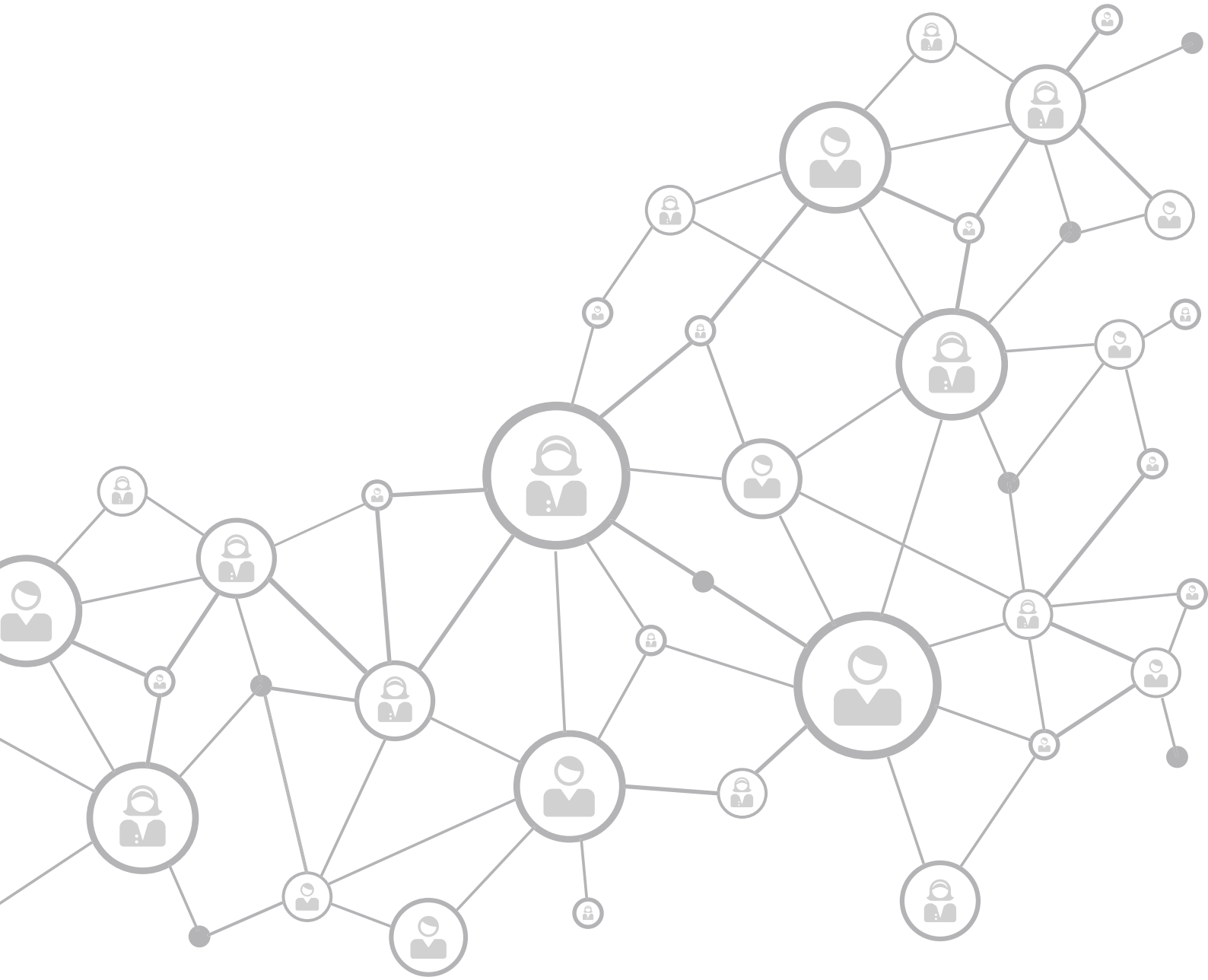
This work has been supported by the RF Government Megagrant 11.G34.31.0048, FP7 ERC PoC 632295 INMOST, Academy of Finland 280700 ABBA, Erasmus+ CBHE 561975 ECOIMPACT.

SUMMARY

- It is widely recognised that in very stable stratifications, at Richardson numbers (*Ri*) exceeding the critical value, $Ri_c \sim 0.25$, turbulence inevitably decays and the flow becomes laminar. This is so, indeed, in the low-Reynolds-number (*Re*) flows, e.g., in some lab experiments; but this is not a hard-and-fast rule. The atmosphere and hydrosphere are almost always turbulent in spite of the strongly supercritical stratification with typical values of Ri varying in the interval $10 < Ri < 10^2$. Until recently, this paradox has remained unexplained.
- The key mechanisms of the seemingly paradoxical self-preservation of the very-high-*Re* geophysical turbulence are (i) conversion of the turbulent kinetic energy unto potential energy and (ii) self-control of the negative (down-gradient) turbulent heat flux through efficient generation of the positive (counter-gradient) heat transfer by the turbulent potential energy (Zilitinkevich et al., 2007, 2008, 2009, 2013). It is precisely due to this loop that turbulence is maintained in supercritical stratifications. Moreover, at $Ri > Ri_c$ the familiar “strong-mixing turbulence” regime, typical of boundary-layer flows and characterised by the practically invariable turbulent Prandtl number ~ 1 (the so-called “Reynolds analogy”), gives

way to the newly discovered "wave-like turbulence" regime (wherein sharply increases with increasing *Ri*), rather than to the laminar regime as is often the case in the small-scale lab experiments.

- It is precisely the wave-like turbulence that dominates the bulk of the atmosphere and ocean beyond boundary layer and convective zones. Modellers have long been aware that turbulent heat transfer in the free atmosphere/ocean is much weaker than the momentum transfer. The new theory has given authentic formulation for this heuristic rule and provided physically grounded method for modelling geophysical turbulence up to very stable stratifications.
- Turbulence is ever present in the atmosphere and ocean and performs the following vitally important "services": (i) transports energy, matter and momentum in the vertical across the fluid geospheres, and (ii) links geospheres via strongly turbulent planetary boundary layers (PBLs) into interconnected climate- and other Earth systems.
- Turbulent mixing is strong in PBLs and very weak beyond PBLs – in the free atmosphere and free ocean. PBLs couple the atmosphere, hydrosphere, lithosphere and cryosphere into a hierarchy of interconnected systems, including the global climate system. PBLs host 90% of the biosphere and the entire anthroposphere (our habitat).
- Convective motions driven by the potential energy of unstable stratification develop over warm Earth surface (or in clouds), and very efficiently transfer heat from the surface upward – thus preventing extremes and moderating thermal conditions at the Earth's surface. Conventional theory, which treated convective mixing as usual turbulence, has got in conflict with modern experimental evidence. Observations of turbulent convection in nature, as well as large-eddy simulation (LES) and direct numerical simulation (DNS) of turbulent convection have revealed, besides really chaotic motions, large-scale self-organised rolls or cells similar to secondary circulations in lab experiments, traditionally considered as artificial, parasitic phenomena. Self-organised convective cells in viscous convection are known since Benard (1900) and Rayleigh (1916), but self-organised rolls have no analogy in viscous convection. They are driven by large-scale turbulent instability caused by the non-gradient horizontal heart flux (Elperin et al, 2002, 2005). Self-organised convective motions are missed in universally recognised theories, such as the heat/mass transfer law: $Nu = 0.14\ Ra^{1/3}$, the Monin-Obukhov similarity theory, etc.
- The shear-free turbulent convection exhibits the following crucially important mechanism disregarded in the conventional theory. Large-scale self-organised convective cell includes the near-surface convective winds towards the plume base. The latter generate mechanical turbulence which, in turn, enhances the heat and mass transfer up to two orders of magnitude.



HUMANITIES & SOCIAL SCIENCES

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Construction of the model change of employment over working age in the Tomsk region, taking into account seasonal fluctuations

SCIENTIFIC ORGANIZATION

National Research Tomsk Polytechnic University

ABSTRACT

The article made modeling the dynamics of change in the number of employed people in the Tomsk region working age. The main aspect of this study is to obtain estimates of the seasonal component additive model that makes it possible to use the data seasonal adjustment in the assessment of income of the older generation, what affects human well-being.

KEYWORDS

Econometric modelling, older generation employment, seasonal fluctuations, human well-being, labor market, seasonal component, employment activity.

SUMMARY

One of the most important areas of study of the problem of well-being of the older generation is to study the activity of the working population of retirement age. A significant factor affecting the labor activity is a seasonal component. The employment of retirees is not constant at different periods - activity is cyclical fluctuations. This is important to study the influence of the seasonal component for the

Simulation of seasonal variation is carried out for the economically active and the economically inactive population of Tomsk region in the working age. The sample set is the data for each month of the economically active population, including employed and unemployed in the period from 2011 to 2013. The seasonally adjusted construction of the additive time series model was chosen as a modeling approach. In the other words each value of the time series is represented as the sum of the trend, seasonal and random components. There is constant oscillation amplitude, so the general view of the model is as follows: Y=T+S+E

Where T - trend component; S - seasonal component; E - random component.

It should also be noted that the most important task in the classical study of economic time series is the identification and statistical evaluation of the main trends in the development of the studied process, detecting the presence of seasonal variations in the range of people of retirement age, and deviations from it. Figure 1 shows the dynamics of the number of employed persons over the working age over the period from 2012 to 2014.

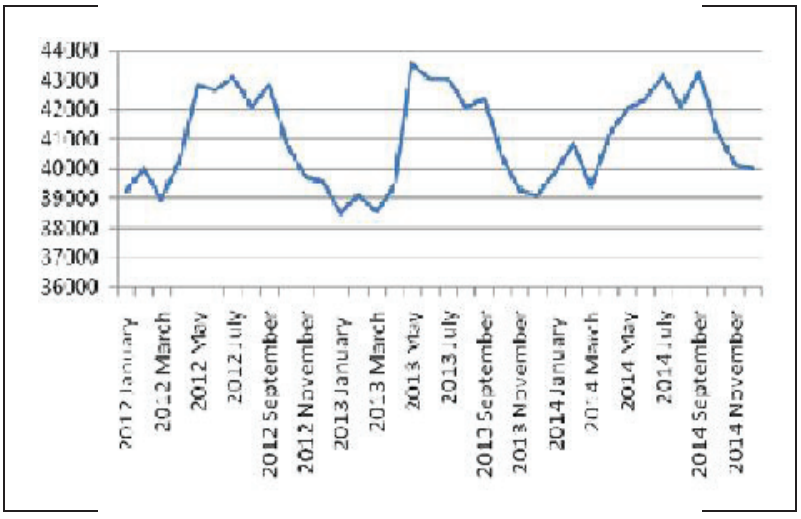

Figure 1. Dynamics of employment over working age in the period from 2012 to 2014

The construction of model changes in the number of employed older generation represents the calculation of all the above components for each time series. The following steps are offered to build this model:

1. Baseline statistics are aligned by moving average;

2. The influence of the seasonal component S on empirical data is calculated;

3. Excluding the impact of seasonality on statistics, analysis of the impact of the trend and the random variable T + E in the additive model;

4. Selection of the best analytical description of the trend component, taking into account the effect of the random component of T + E;

5. Trend and random components are calculated in the model;

6. Forecast values of deferred employed people over the working-age population with the resulting model.

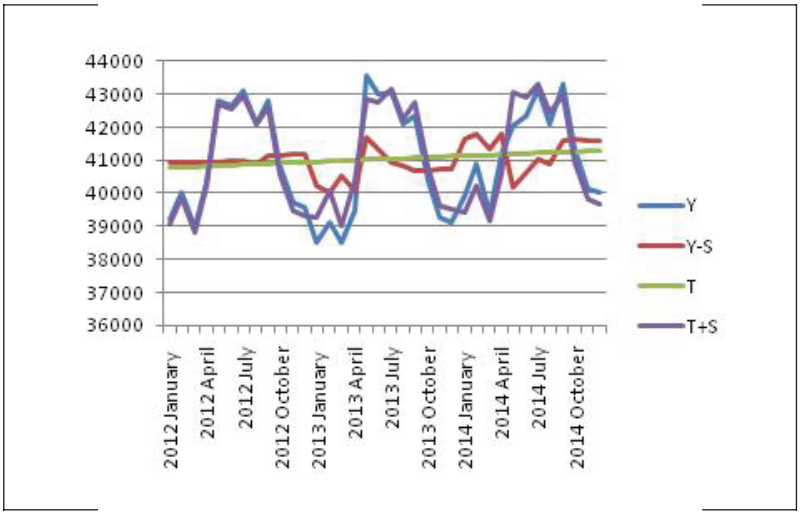

Figure 2. Changes in the statistics, the data with the excluded impact of seasonal and random components, as well as the trend of employment of the elderly population of the Tomsk region

When analyzing the data of the economically active population of working age, seasonal variations with frequency of 12 were shown, because the number of employed people is much higher in July than in January. Thus, the analyzed factor reaches a peak in winter and summer.

Excluding the impact of the seasonal component and subtracting its value from each level of the original time series, we obtain the value T + E = Y-S. In this case, the data contain a trend component and a random component only. Fig. 2 shows the dynamics of these components of the indicator changes in the employment of the elderly population: the original data Y, data with excluded the impact of the seasonal component Y-S, data with excluded the impact of random components T + S, trend component T only. Figure 3 shows the quantitative impact of seasonal and random components for each moment all the time during the analyzed period.

Dynamic of statistics is showing the impact of the magnitude of the seasonal component in the overall level of employment. Curves Y and YS have a slight resemblance - the maximum level of influence of the seasonal component is close to 2,000 jobs. This random component has little effect on the overall activity of the population of working age. Curves Y and S + T are almost the same - the maximum level of influence of the random components does not exceed 1000. Therefore, we can conclude that the degree of influence of seasonal variation than the random variable 2 times.

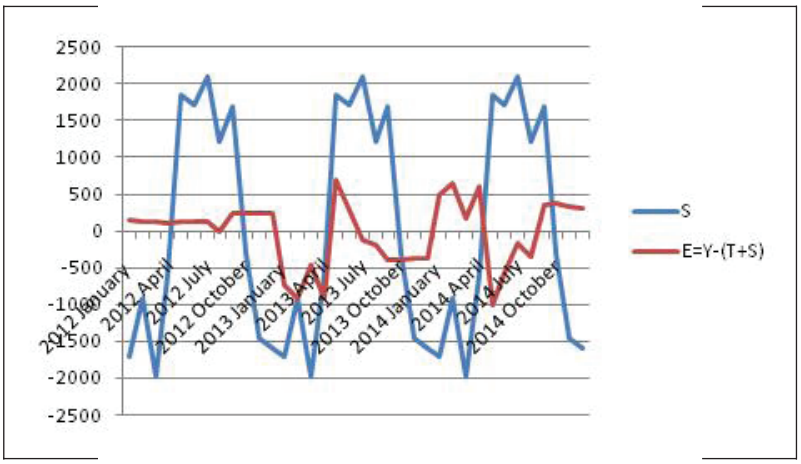

Figure 3. Dynamics of seasonal and casual component in the analysis of the employment of the elderly population

Figure 3 shows the dynamics of changes in the seasonal and random components in the overall level of employment of persons older than working age. Thus, it can be concluded that the maximum value of the random component of the absolute value is approximated to 1500. The impact of the seasonal component in the overall level of economic activity of pensioners in absolute value exceeds 4,000.

It is necessary to align the analytical series T + E by a linear trend to determine the effect of directly trend component T. Substituting in this equation the values t = 1, 2, ..., 16, we find the levels of T for each time point, substituting the values t = 1, 2, ..., 16 in this equation. We can find the value of a number of levels obtained by the additive model. To do this, it is necessary to add the values of the seasonal component for the respective months to the levels of T.

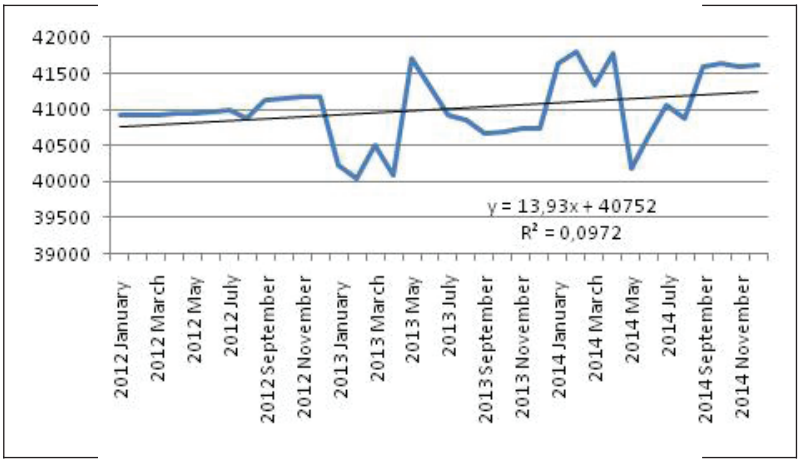

Figure 4. Changes in employment over working age after excluding the seasonal component for the period from 2012 to 2014

Figure 4 shows the dynamics (after excluding the seasonal component) and the trend of the economic activity of the population of retirement age. The trend looks upward straight y = 13,93x + 40752. There has been an increase in the activity of the slow pace of work - the number of employed persons over the working age increased by only 1% for two years.

An important component is the comparison of the initial statistical data and data after excluding the impact of the random component to identify the seasonal fluctuations in employment over working age. On the same graph we should postpone the actual values of levels of time series and theoretical received under an additive model.

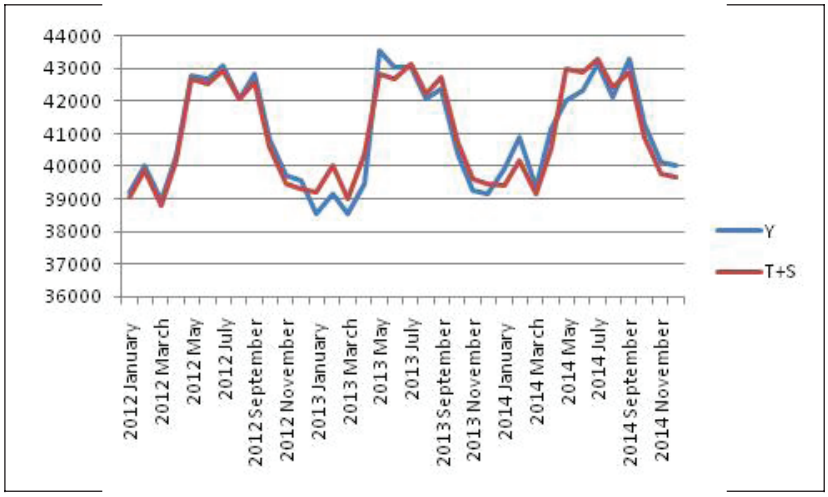

Figure 5. Dynamics of changes in employment over working age (the original data and the data with eliminated the random variable)

Random component in the total number of employed persons over the working age does not exceed 1,000 jobs.

We should apply the method of the sum of squares obtained the absolute errors to assess the quality of the constructed model. The coefficient of determination is equal to 0.922102183. Thus, we can say that the combined model has built 92% of the total variation of levels of time series of the number of employed people over the working-age population.

According to the results of this work there are following conclusions:

1. Modeling the dynamics of change in the number of employed people over working age allowed to obtain estimates of the seasonal component under the additive model. For example, with an annual increase in employment of 0.5% must be taken into account that in July of each year, increasing of the number of jobs in 2000 are required due to the increase of labor activity.
2. This makes it possible to use the data seasonal adjustment in the assessment of income of the older generation, which in turn affects the welfare of the population.

The ratio of the labor market in the region are increasingly will be determined by the social activity and social mobility of persons older than working age. The package of measures to preserve their economic activity takes into consideration the influence of the seasonal component in the overall level of activity of people of retirement age. In a situation of decreasing working-age population important activity seems to maintaining employment and social activity of the elderly generation.

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Social Capital in Russia

SCIENTIFIC ORGANIZATION

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ABSTRACT

Based on the World Values Survey (WVS) and Putnem`s definition of social capital the current study covers the period from 1990 to 2011. WVS data demonstrates that after a significant decrease in 1995 generalized trust is slowly recovering while membership in civic associations remains rather stable over the past 20 years. At the same, time Russians are becoming more and more tolerant towards different types of anti-social behavior including bribe-taking, avoiding a fare on public transport and claiming government benefits which a person is not entitled to.

KEYWORDS

Generalized trust, civic activity, prosocial attitudes, World Values Survey.

ACKNOWLEDGEMENTS

The study was funded by Russian Foundation for Basic Research, grant № 16-36-00372 «Formal, Informal and Familiaristic Social Capital: Cross-cultural Analysis with Multilevel regression modeling».

SUMMARY

Social capital has become one of the most debatable and popular concepts in social sciences. As A. Portes notes it «has evolved into something of a cure-all for the maladies affecting society at home and abroad» (Portes, 1998: p. 2). Indeed,

recent studies demonstrate positive correlation between economic development, well-functioning civic and political institutions, high quality of life and different dimensions of social capital (Knack, Keefer, 1997; Zak, Knack, 2001; Beugelsdijk, Groot, Van Schaik, 2004; Inglehart, Welzel, 2011; Rothstein, Uslaner, 2005; Tokuda, Fujii, Inoguchi, 2010).

There are many approaches to definition of social capital, but one of the most widely used ones belongs to R. Putnam who treats it as «features of social organization, such as trust, norms and networks, that can improve the efficiency of society by facilitating coordinated actions» (Putnam et al., 1994). Following this idea, scholars divide social capital into three main concepts: 1) generalized trust which relates to strangers and out-groups: 2) civic activity; and 3) prosocial norms and behavior. Though the first two elements have been extensively studied during recent decades (see Nannestad (2008), Stolle (2002), Musick & Wilson (2008)) the third one has remained underinvestigated.

There is a stereotype that after the collapse of the Soviet Union social capital significantly dropped. The current study aim to test this suggestion and trace three mentioned elements of social capital for the period from 1990 to 2011. The data is based on the World Values Survey (WVS) and the European Values Study (EVS). The Russian Federation participated in four waves of the WVS (1990, 1995, 2006 and 2011) and in two waves of the EVS. In 1990 data was collected only in Tambov.

Generalized trust is captured by so called standard trust question «Generally speaking, would you say that most people can be trusted or that you need to be very careful in dealing with people?» It has a dichotomous scale and two possible answers: 1) most people can be trusted and 2) need to be very careful. Although this way of measurement has been severely criticized because of the trust radius problem (Delhey, Newton, and Welzel 2011; Sturgis and Smith 2010) this is the only indicator available since 1990. The more advanced question on generalized trust – question about trust in people one meets for the first time – was for the first time included in the 5th wave of the WVS.

According to the WVS and EVS data in 1995 generalized trust decreased from 37 % in 1900 to 24%. After that it had been recovering and reached its highest point in 2008 when 30% of respondents answered that most people could be trusted. Compared to 2008, in 2011 trust remains almost at the same level.

Civic activity is operationalized through formal membership in four types of associations (sport or recreational organizations; art, music or educational organizations; environmental organizations; professional associations) and signing petitions. It is worth noting that the share of people who belong to such organizations has been rather stable during past 20 years: from 2% to 6%. The only exception is the slight rise which took place in 2006. Sport, recreational and cultural organizations were the most popular ones during that period while environmental organizations had the lowest number of members. Turning to the average membership per person it ought to be mentioned that this indicator also demonstrated a quite stable trend. In 1990 around 11% of respondents belonged to at least one of these organizations, in 2011 this statistic did not changed.

To capture direct form of participation WVS asks if a person signed a petition or could do this in the future. WVS and EVS show that this type of civic activity has a downward trend. While in 1990 30% of respondents did sign a petition, in 1995 only 11% of respondents answered this question positively. The potential activity demonstrates similar decline. However, there were no statistically significant changes between 2006 and 2011 that could be considered as a positive tendency.

The last dimension of social capital is prosocial norms and behavior. Unfortunately, WVS and EVS do not ask about such behavior directly but they have a battery of items which relates to the attitudes towards prosocial/anti-social behavior. It includes justification of the following practices:

1. Claiming government benefits to which a person is not entitled to;

2. Avoiding a fare on public transport;

3. Cheating on taxes if a person has a chance;

4. Accepting a bribe.

All items have 10-point scales which were recoded to dichotomous variables (1 («never justifiable») relates to strong rejection; points from 2 to 10 relate to acceptance of such behavior).

Analysis reveals that bribe-taking was the most serious violation while avoiding a fare on public transport was justified by a largest number of respondents. Unfortunately, Russians are becoming more and more tolerant towards these types of anti-social actions. Between 1990 and 2011 the share of people rejecting bribe-taking, claiming government benefits and avoiding a fare has been constantly decreasing (from 85% to 65%, from 65% to 42%, From 52% to 30% correspondingly). The declining trend in the justification of avoiding taxes is less pronounced.

Summing up, it is possible to draw several conclusions. First, generalized trust has reached almost the same level as it was before the collapse of the Soviet Unioun. Second, over 20 years formal membership has been rather stable while the number of people who signed any kind of petition or ready to do it has declined. Third, attitudes towards anti-social behavior has becoming more positive indicating the erosion of social norms.

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Applying sociological approach to studying older people's well-being

SCIENTIFIC ORGANIZATION

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ABSTRACT

An important tendency in the development of the recent research of the problem concerning older people's well-being is studying not so much the objective indicators of economic and social development as the subjective anticipations and preferences whose aggregation enables to obtain a more complete picture of reality through the prism of subjects' attitude to what is going on. This task can be handled with the application of the questioning technique. Practice of social approach to studying the problem of well-being has been analyzed and its necessity has been reasoned.

KEYWORDS

Social research, older people's well-being, well-being factors, well-being indicators.

ACKNOWLEDGEMENTS

This work was performed by the author in collaboration with Tomsk Polytechnic University within the project in Evaluation and enhancement of social, economic and emotional wellbeing of older adults under the Agreement No.14.Z50.31.0029.

SUMMARY

Studying well-being aspects was based on the devised evaluation method, which includes the social research method. Application of the sociological approach allowed studying well-being from the perspective of real status of a person in different spheres of life; from the standpoint of perceiving this status and the level of satisfaction; through the spectacle of perceiving objective living conditions in society including those which are directly related to satisfying the requirements of the people belonging to the "third age" (the quality of health service, accommodation, housing and utilities services, social security and social services; the level of income and priorities in spending money; consumed services; leisure activities; societal problems older people are concerned about, etc.); from the standpoint of emotional disposition and vision of the future.

The process of detecting and forming the system of factors influencing the level of well-being consisted of five stages. The first stage was devoted to selecting significant factors reflecting the major processes, then there were determined the assumptions required for simplifying the process of detecting and forming the system of external factors influencing the level of the older people's well-being. At the third stage the well-being was evaluated on the basis of the distinguished factors. Afterwards, there were suggested the hypotheses and supposition concerning the cause-and-effect relationship between the factors and well-being of the people

falling into the category of the “third age”. And, finally, the analytical procedure was finalized by drawing conclusions.

The basic condition for choosing indicators was represented by the direct link between an indicator (action) and the characteristic which this indicator must detect. The more sensitive indicators possessing a more precise accuracy grade were chosen from the group of indicators characterizing the subject of research. When building the indicators, there were taken into account the objective and factual data and subjective feelings as well as international experience of measuring the standards of living in the developed countries, particularly, the key indicators of Active Ageing Index for age groups (level of employment, participation in public life, independent and safe living, opportunities for active ageing).

The major research method applied was questionnaire survey conducted by means of semi-structured interview. The opinion surveys form which was approved during the pilot studies in 2014 and completed with regard to the results of the research conducted in 2014 was used. The form included the questions on the following key blocks of socio-economic and emotional well-being: economic status, health and medical support, physical activity, social activity, using information technologies in everyday life, life satisfaction.

The measurement method includes simple, direct evaluation techniques based on using single questions and scales. The form was developed on the bases of nominal and ordinal scales. Application of scaling technique enabled to quantify the values, characterizing the process under research, assign numerical and symbolic series, and consider the degree, quantity and frequency of manifestation of the event under investigation collectively and separately. The following event was quantified: economic, social and emotional well-being. The subjective distinction acted as the unit of measurement.

Well-being measures of quality indexes were determined with regard to the requirements within the social parameters comprising integrated values and reflecting the sense of being successful or unsuccessful; unambiguity of interpreting the parameters being set by the respondents belonging to different age groups; accommodation of changes in the standard of living. Proving the reliability of indexes (points) and scales was made with the accordance to the internal consistency on the basis of Cronbach’s alpha and splitting coefficients. The form includes screening questions aimed at checking the respondents’ answers unambiguity.

The method of combined sampling was used for selecting survey units. The sampling mentioned is based on the following principle: routing sample (survey initial points were assigned); quota sample (control values quotas are proportionate to the parameters of the general population with regard to gender, age and place of residence).

General population is represented by people who are 55 years of age and older and live in Tomsk region. The size of general population is 229000 representatives (according to the results of the Russian Census of 2010), 154300 of them live in cities and 74680 live in the country. With the stated size of general population it is sufficient to survey 400 people (calculation was carried out on the basis of confidential interval formulae by using the following calculator http://www.fdfgroup.ru/?id=189). Under condition of the given size (400 persons) the sampling error (standard deviation) on the grounds of control values with confidence probability (accuracy) equal to 95% falls within the limits of ±4.9%, i.e. in case of conducting 100 research with such kind of sampling, 95% of the answers, according to the law of statistics, will range within ±4.9% from the initial one. Confidence probability is 95%, which complies with the practice of conducting sociological research in Russia and international community.

Gender and age distribution (statistical values) in sampled population corresponds to the parameters on these characteristics in general population. When calculating the sampling on the ground of gender and age the results of the Russian Census of 2010 were applied. Gender structure reflects the general situation in Russia, i.e. the correlation of older men and women is 1 to 2 respectively. Gender and age distribution (statistical values) in sampled population corresponds to the parameters on these characteristics in general population.

The subject of research was averaged out on the grounds of gender, age, place of residence, educational background, and employment. Furthermore, the subject of research was averaged out on the following grounds: optimism/pessimism, life satisfaction, and predominant emotional disposition with the purpose of hypothesis justification.

On the basis of research outcomes there was created *the profile of an average pensioner living in Tomsk region.*

An average pensioner is described as follows: a 60-65 years old woman living in a city, married or widowed, with secondary vocational education, a former employee. She is currently unemployed but owns a home garden, which is an additional source of getting food, place of spending free time (a hobby) and method of following family traditions simultaneously. The need for labour is expressed in the intention to work on the personal home garden.

Generally, the obtained results complement the database of older people's well-being indicators. The database was established in a laboratory and is applied for studying the impact of various factors on life satisfaction and behavior of older people in the mentioned region.

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Business Policemen behind the Blue Veil of Silence: Determinants of Centrality and Law Enforcement Outcomes in Corrupt Elite Networks

SCIENTIFIC ORGANIZATION

Higher School of Economics

ABSTRACT

This study seeks to understand why certain corrupt actors are more central than others, and how personal centrality in a corruption network affects the probability of law enforcement outcomes, whistleblowing, and assassination. To address these questions, we draw upon organizational and covert networks theories and use documentary and archival data to reconstruct the actual cooperation networks involved in high-profile police corruption in Australia, Bulgaria, Canada, China, Russia, the United Kingdom, and the United States.

KEYWORDS

Corruption, police, covert networks, sentencing.

SUMMARY

Public sector corruption is a large 'industry' generating annually about US $1 trillion dollars in bribes (World Bank 2004). For 'corruption enterprises' to be financially successful despite institutional change, they must possess an intelligently-designed production technology organized around talented leaders able to recruit capable, trustworthy criminal minds effectively blocking any anti-corruption investigations and reforms. However, criminal networks face a trade-off between secrecy and efficiency (Morselli 2009; Crossley et al. 2012). More central players have more associates, are involved in more criminal activities, and thus are more visible. Therefore, an actor's location in a criminal network should influence the likelihood of penalties (Baker and Faulkner 1993). Different crime cultures exhibit different modus-operandi, and social structure (Morselli 2009). Elite corruption differs from ordinary (serious and organized) crime (Gambetta 2000; Varese 2000; Lauchs and Stains 2012). Corrupt top policemen, having a monopoly over violence and coercion and operating within a paramilitary bureaucracy, have different incentives to form ties from ideology-driven terrorists, politically-motivated mafiosi, or profit-seeking criminals.

Given the understudied field of organized elite police corruption and its deleterious consequences for socioeconomic development (Ivkovic 2005; Johnston 2005) and (inter)national security (Gerber and Mendelson 2008), this study seeks to understand: 'Why are certain actors more central than others?', and 'How does an actor's point centrality in a corrupt network affect the probability of law enforcement outcomes (allegation, arrest, verdict, and sentence), murder (death sentence or gun-justice), and whistleblowing (whistleblower or supergrass)?' To address these questions, we draw upon organizational, organized crime and covert networks theories and use documentary and archival data to reconstruct the actual cooperation networks involved in high-profile police corruption in Australia, Bulgaria, Canada, China, Russia, the United Kingdom, and the United States.

Although aspects of 'covert,' 'conspiracy,' 'clandestine,' 'shadow,' 'underground,' 'illegal' or 'dark' networks have been studied by organizational criminologists and network analysts (e.g., Morselli 2009; Xu and Chen 2010), the elite corruption's structure, leadership characteristics, and effect on outcomes have remained virtually unexplored (Launch et al. 2011, 2012). Moreover, there is a lack of comparative 'networked' corruption research. The study of organized, high-level corruption is important for both theory and policy. We contribute to secret societies, covert networks, organized crime, and organizational theories by studying elite illegal networks comprising public servants and their clients. Identifying the socioeconomic characteristics of highly successful corruption entrepreneurs, and exploring the web of their hidden interactions, may allow us to design better anti-corruption policies. Last but not least, our study explores the extent to which theories based on legal, secret or criminal networks are generalizable to corruption.

We applied theoretical sampling (Eisenhardt and Graebner 2007) selecting well-documented, high-level, organized police corruption with the different main corrupt activities in different nation-states. Our corrupt police networks include: the Australian 'First Joke' (1959-1974), the Bulgarian Prime Minister Boyko Borisov's corrupt network (1990s-2015), the Canadian 'Ontario Provincial Police Union Scandal' (2015), the Russian Chayka Family (2016), the British 'Groovy Gang' (1990s-2000) and 'Operation Nightshade' (1993), the U.S. 'L.A.P.D. Rampart Scandal' (1990s-1998), and the Chinese ex-security chief Zhou Yongkang's guanxi (1998-2012).

We hypothesize that actors of higher socioeconomic status, criminal reputation and the ability to uphold the secret code, will be perceived more valuable, trustworthy partners in crime, will attract more criminal associates, and thus will be more central. We suggest that former members of political or secret organizations, having greater symbolic and social capital (Bourdieu 1997), are more likely to be sought as brokers between the police and (il)legitimate networks or organizations. We expect that males and particularly close family members, being considered more trustworthy in the uncertain criminal world (Abadinsky 2007), will be part of the boss's inner circle. We predict that more central actors, having greater involvement in corrupt activities, will face stiffer criminal sentencing. Brokers and middle managers, possessing sensitive information and experiencing greater performance pressure, will be more likely to be lobbied by the police and become informants. However, the latter are also most likely to be murdered by the corruption boss. Lastly, we hypothesize that top officials, being able to better buffer themselves, will receive more lenient criminal sentencing.

ADDITIONAL INFORMATION

Ivan Aymaliev, PhD Candidate, is a Junior Research Fellow in criminology at the Higher School of Economics (HSE), Moscow, Russia. His academic background is in economics and sociology. He has degrees from the University College London (UCL), UK, and the HSE. His research interests include corruption, police, and covert networks.

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Western Innovations and Monarchist Ideologies in Political Culture of Imperial Russia

SCIENTIFIC ORGANIZATION

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ABSTRACT

The paper deals with the important problem of the origins and influence of Russian monarchism. While researhers usually describe moanrchism as a bulwark of traditionalism, it could be seen a dynamic phenomenon, which facilitated the whole process of intellectual and cultural transfer from Europe to Russia. There were 3 major fields in which the monarchical ideologies were developing: the providential, the historical and the modernizing. The combination of these 3 approaches to monarchy shaped the phenomenin of monarchism as paradigmal for political thought of Imperial Russia.

KEYWORDS

Monarchism; innovations; Russia; ideology; cultural transfer.

ACKNOWLEDGEMENTS

The paper was prepared with the support of the grant of Government of Russia for attraction of the leading scientists to Russian institutions of higher learning, research organizations of the governmental academies of sciences, and governmental research centers of the Russian Federation (project 'Return to Europe: Russian elites and European innovations, norms and patterns (18 - beginning of 20th centuries)', Ural Federal University, contract № 14. A 12.31.0004).

SUMMARY

Monarchism is typically thought of as an element of tradition, which was to be replaced by the European innovations like constitutionalism, liberalism or republicanism. However, while studying the sources in Russian political thought of 18th - early 20th centuries, we might find out that monarchist ideologies were able to react in a flexible way and to appropriate the results of the intellectual transfer from the West. We can speak of 3 main modes (fields) or ideologies of monarchism that were historically deployed in Imperial Russia. First, it is the providential ideology, which was an amalgam of Russian Orthodox providentialism and new European baroque strategies of comparing the Czar to God. Second, it is the historical approach, which emerged in the middle of 18th century. Its centerpiece was the political glossary of Aristotelian philosophy, the language of the forms of government. History and political science within this ideology could demonstrate that monarchy was the best form of government for Russia (such was the mainline for Russian historicans from Tatishchev to Karamzin and later on). On this basis, the 19th century nationalist were able to fuse the historical monarcist ideology with the nationalistic vision of Russia's uniqueness in history. Third, it is the concept of monarchy as an agency of modernization. This ideology was emphasizing the under-developed state of Russia (and, not least, the backwardness of the majority of population, namely peasants); to overcome it, a benevolent rule of the monarch is required.

A combination of these three ideologies provided Russian monarchism with a sustainability; monarchism proved great historcal endurance. That also meant that serious alternatives to monarchist ideology were forced to employ radical ideas to be able to penetrate into the monarchical stronghold of political thought.

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SCIENTIFIC ORGANIZATION

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Technologies for active lifestyle in later life: design and evaluation

ABSTRACT

This paper explores the impact on social interactions on adherence and effectiveness of home-based physical training programs for older adults. We describe the design of a system for home-based intervention that enables older adults with different abilities and indeed in spite of their different abilities, to engage in group exercises from home, via a tablet, while keeping these differences invisible to the group. We then report on interventions run with dozens of subjects in different countries, reporting on the outcomes related to physical, psychological and social wellbeing.

KEYWORDS

Wellbeing, physical training, older adults.

ACKNOWLEDGEMENTS

This work was supported by the project "Evaluation and enhancement of social, economic and emotional wellbeing of older adults" under the agreement no. 14.Z50.310029, Tomsk Polytechnic University.

SUMMARY

Background

Engaging in physical activity can bring multiple benefits to the health and well-being of older adults. It reduces risk of falls, slows progression of degenerative diseases, and even improves cognitive performance and mood [1].

There are however a variety of barriers that make it difficult for older adults to engage in regular physical activity: lack of adequate facilities and infrastructures, reduced functional abilities, lack of motivation, and in general, the simple reason that it is no longer easy to leave their homes and participate in physical activities on a regular basis. Thus, and in spite of the growing evidence of the benefits of physical activity, as well as the adverse effects of sedentary behavior, physical inactivity is still prevalent in older adults [2].

Intervention programs to promote physical activity in older adults, either in group or individual (home) settings, have demonstrated the potential to improve health and functional performance [3]. Both types of intervention have shown equivalent health outcomes but with different results when considering adherence. Group-based interventions seem to achieve higher participation in the long-term, while in the short-term the results are comparable or not conclusive. However, there are many factors that can make group exercises a challenging (or infeasible) setting for older adults. A major obstacle, due to the heterogeneity of this broad population, is the big difference in the level of physical abilities between participants: unless the training class is tailored to the needs and abilities of each group, we are likely to see limited effectiveness as well as lack of motivation in performing the exercises [5], which proves itself difficult in heterogeneous groups. This difference in physical abilities, along with the logistic and practical obstacles that make it more difficult, as we age, to regularly attend a gym and perform group exercises, means that, for some adults, home-based individual intervention is the only viable training option.

In this paper we report on a technology-based physical intervention that enables older adults with different abilities, and indeed *in spite* of their different abilities, to engage in group exercises from home while keeping these differences invisible to the group. The intervention is based on the OTAGO Exercise Program for fall prevention [6] and supported by a set of applications that allow older adults to follow virtual training sessions via a tablet device under the supervision of a remote coach. Different interventions were performed, in different contexts, different target groups, and different countries. In this paper we report on a specific internvention, including a total of 37 adults aged between 65 and 87 years old (28 females and 9 males, mean age = 71, sd = 5.8) that followed a personalized home-based strength and balance training plan for eight weeks. The participants performed the exercises autonomously at home using the Gymcentral application. Participants were assigned to two training groups: the Social group used an application with persuasive and social functionalities, while the Control group used a basic version of the service with no persuasive and social features. We further explored the effects of social facilitation, and in particular of virtual social presence, in user participation to training sessions. The main outcome measures were adherence, persistence and co-presence rate, and we also assessed physical and psychological wellbeing as well as behavior change.

Previous studies have demonstrated effectiveness of the OTAGO Exercise Program in reducing falls and fall-related injuries among high risk individuals, and increasing the percentage of older adults who are able to live independently in their community [6]. Although this specific program was designed for home-based training, a meta-analysis including other exercise programs for fall prevention found that combining group-based and home-based exercises is a strategy used in several effective trials, thus recommending both options to be available [7].

Technology-based interventions have also demonstrated to be effective in increasing and maintaining physical activity [8]. Among the technological components that have been explored we can mention: online newsletters [9], personalised emails [10], web-based videos [11], tablet applications [12] and video game consoles [13]. However, most of the existing intervention studies have focused on individual training, or provided a social context that was limited to forums or chats [14]. Even exergames, a type of technology that have traditionally provided more immersive experiences (e.g., via MS Kinect and Nintendo Wii), have not been explored in an online group setting.

A Virtual gym for older adults

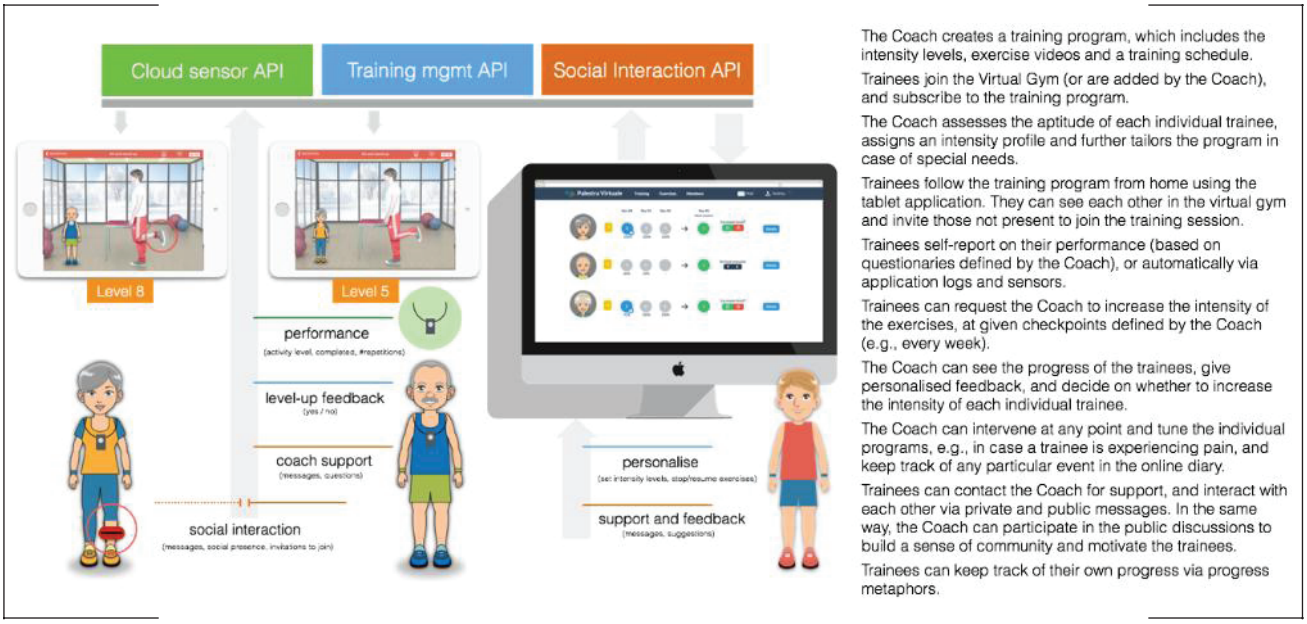
Gymcentral is a software designed to enable and motivate independent-living older adults - of potentially different abilities - to follow group exercises from home, relying on social interactions both as a motivation and as an end themselves.

The design of Gymcentral is informed by evidence in the literature as well as previous experiences that shaped the current implementation of the application. Active Lifestyle and its successor, the Virtual Social Gym, explored the feasibility of providing a home-based strength and balance exercise program by means of video exercises in a tablet device [12]. In addition, it studied the effects of using individual (e.g., positive and negative reinforcement) and social persuasion strategies (e.g., collaboration and competition) in the adherence to the training programs.

Based on this early work and the feedback we obtained, we developed a software application that enables home-based training and that i) includes *tailored* exercise programs, ii) includes the possibility of interaction with a human coach, and iii) performs remote monitoring by employing an activity monitor in the context of a home-based physical intervention. In addition, we wanted to experiment the possibility of older adults of different abilities, and indeed *despite* this difference, to engage in (virtual) *group* exercises from home while keeping disparities invisible to the group. Thus, we explored different design alternatives to realise the group exercising (see Figure 1c.), from simply indicating that another trainee was also training (online status) to having a real-time motion and visualisation (3D and motion), each alternative with a different level of immersion, feedback and requirements in terms of technology.

Figure 1. Training applications. a) Active Lifestyle app, exploring the use of individual and social persuasion strategies; b) Virtual Social Gym, exploring the use of activity monitors in home-based interventions; c) Gymcentral early design alternatives; d) Gymcentral application in its current form.

Figure 2. Gymcentral application workflow



The design alternative materialised in the current version of the tool (Figure 1d), relies on the virtual environments, which have been shown to increase the sense of presence, or psychological immersion. In addition, social presence, along with user embodiments (avatars), helps to reduce physical barriers and get users more engaged in the activities while preserving their privacy. Avatars however do not follow the actual trainees movement but predefined movements. This was both a practical constraint (i.e., to keep the technological requirement to a minimum) and a design constraint (i.e., to keep the specifics of the exercise performed hidden from others).

The Gymcentral platform is organised in two main applications that serve the needs of both trainees and the coach. Older adults can follow the training programs by using a tablet-based application and sensors, and the coach can monitor the entire coaching process from a web-based application (Figure 2).

STUDY

Design and Setup

The main objective of the study was to understand if social presence increases adherence to an exercise program. Secondary objectives were to assess effect on physical wellbeing, social wellbeing and behavior change. The study followed a framework for the design and evaluation of complex interventions in health settings [Campbell et al., 2000]. Using a random assignment procedure, participants were assigned to an experimental (or social) condition and to a control condition, considering *age* and *participants' frailty level* as the random assignment variables.

Participants in the social group were given a version of the Trainee App that included the personalised training program, social environment for group exercising, messaging and persuasion features. Participants were aware that they were exercising together and they could choose to do so. In the control condition, participants received a version of the application that focused only on the home-based program, delivering the personalised training but without social or individual persuasion features. Participants were offered three training modules (~1.5 hours each) focusing on operating the tablet, the use of the main applications and the Gymcentral app.

All participants underwent physical assessment with a personal trainer before starting the exercise program. This allowed for personalised tailoring of exercise type and intensity, and for personalisation of the starting level of each participant. Enjoyment of physical activity was also measured, using the Physical Activity Enjoyment Scale [PACES; 4], to test for differences that might favor the participation in one of the groups. An analysis of variance however showed no significant main effect for the groups ($p = .477$).

The study took place over a period of 10 weeks. The first week was devoted to technical deployment and application testing, followed by 8 weeks of training and 1 week of post-training measurements. The training program was supervised by a training coach, who could intervene to advance trainees in the exercise program, and to provide technical support upon request. No differences in support related to the app were registered.

The exercise program implemented in this study was developed on the basis of the OTAGO Exercise Program [6], and was adapted with by a professional personal trainer in order to fit the original program into 10 levels of increasing difficulty. The study received ethical approval from the CREATE-NET Ethics Committee.

MEASURES

Following several threads of previous work, we measured:

- Attrition
- Adherence
- Physical ability based on commonly adopted tests such as *30-second chair* stand and *get up and go*, to assess muscle strength and gait speed
- Enjoyment, using the PACES scale [4]
- Wellbeing, using the Wellbeing scale of the Multidimensional Personality Questionnaire [MPQ; 15]
- Processes of behavior change. One theory that has been recently applied to the study of persuasive technologies is the Trans Theoretical Model of Behavior Change [TTM; 16].

RESULTS

Attrition. The intervention resulted in a 7.5% attrition rate, measured in terms of the proportion of participants lost at the end of the study. Reasons behind the withdrawal of these participants were related to unexpected health and family problems or, in one case, because of Internet connection issues which could not be solved.

Persistence (fig 3). In the social group the persistence rate was 85%, while in the control group it was 64%. A t-test for independent samples showed that the social group had a significantly higher persistence rate (M=85.4%, SD=16.1%) compared to the persistence rate of the control group (M=64.2%, SD=24.1%), t(35)=3.18, p=.003).

Strength and speed (fig 4). Both groups showing a significant improvement in the test assessing leg muscle strength,(F(1, 33)= 19.275, p < .001, partial eta squared = .369), with with participants in the social group performing significantly better despite non-significant differences in prior conditions. In terms of speed, multiple comparison tests with Bonferroni correction showed that gait speed significantly improved for the Social group (p = .002) but not for the Control group (p = .285).

Enjoyment and **wellbeing** both improved, but we did not see any significant difference among the groups.

Participants in the Control group have experienced an increased usage of some of the **processes of change** such as counterconditioning, reinforcement management, self-liberation, social liberation, which can be attributed to an increased awareness about the benefits of physical

activity as a result of the intervention. In the Social group, participants have also increased in consciousness raising, dramatic relief and self-reevaluation.

Figure 3: adhrence to the program

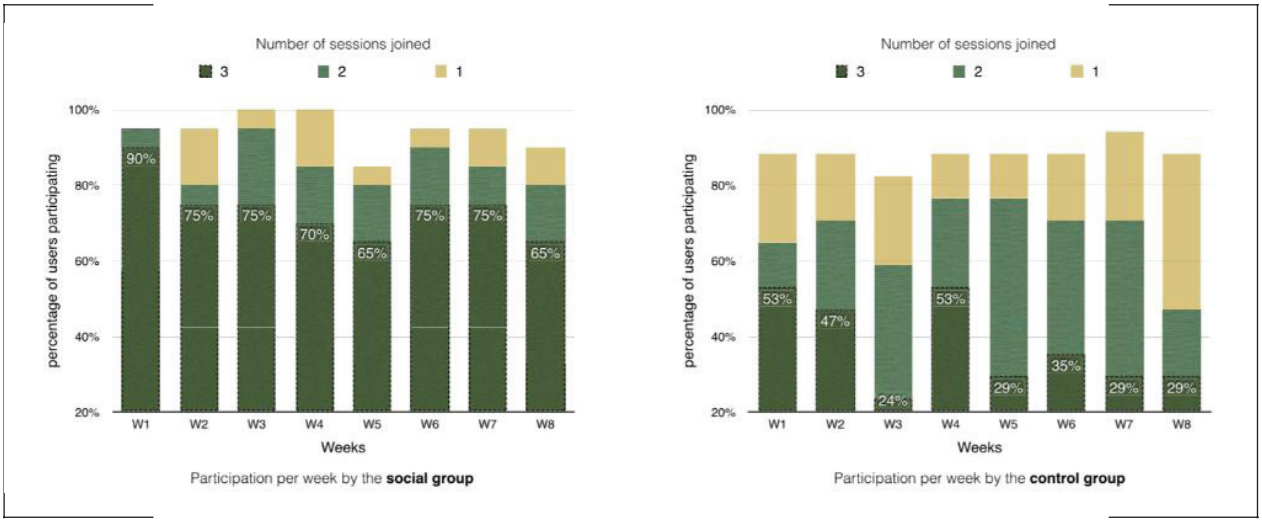
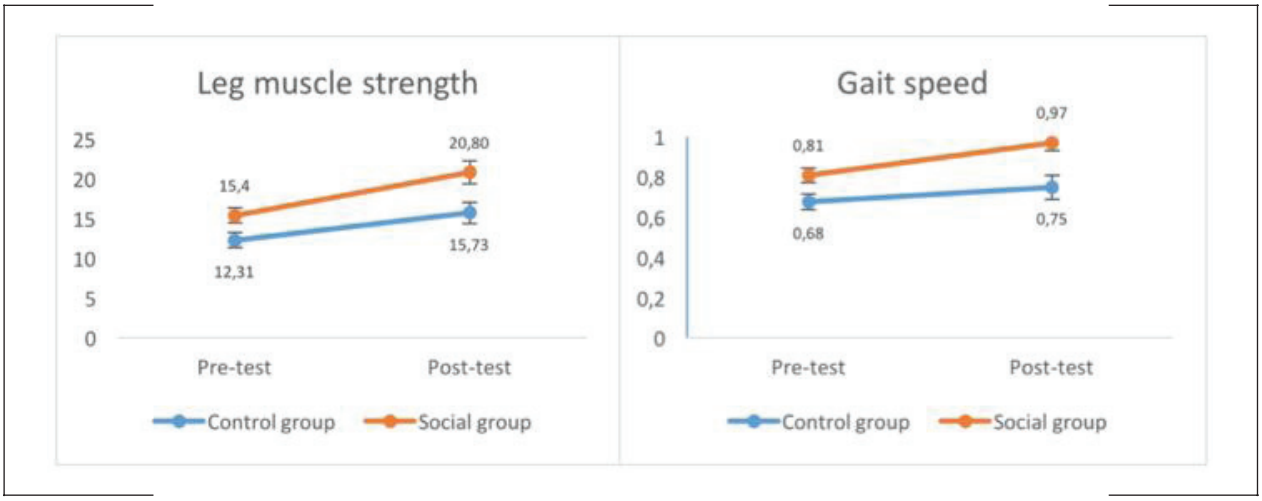


Figure 4: muscle and speed improvements



MAIN FINDINGS

The main finding we take home from the study is the impact on group exercising, both in terms of adherence and results. Furthermore, participants did prefer to train in group, as we witnessed a clear tendency for people to train (virtually) together when possible.

We also observe that virtual training programs, and specifically group-based ones, are effective in triggering the process of change. One of the most striking examples of this is that months after the end of the trial the participants came back to ask to reactivate the platform permanently, which we did, and bought their own tablets and internet access to keep exercising.

Longer studies with more participants are instead needed to assess the potential for effects on wellbeing and differences among the groups.

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Subjective wellbeing in older adults living in Tomsk Region

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ABSTRACT

This study investigates the subjective wellbeing of older adults living in Tomsk Region. We administered 2 questionnaires. In each questionnaire 600 respondents (aged 65 years or over) were interviewed face-to-face. We evaluated how life satisfaction is affected by demographic factors (eg., age, gender, etc.), social aspects (e.g., social network, isolation and comparison, etc.), psychological characteristics (e.g., depression, dispositional optimism). Both questionnaires provided new and interesting insights about the subjective wellbeing of Siberian older adults.

KEYWORDS

Survey; Cross-sectional study; Subjective wellbeing; Life satisfaction; Older adults; Tomsk Region.

ACKNOWLEDGEMENTS

This study was supported by the project “Evaluation and enhancement of social, economic and emotional wellbeing of older adults”, under the agreement No.14. Z50.31.0029, Tomsk Polytechnic University.

INTRODUCTION

Twenty-eight percent of the Russian population will be aged 60 years or over by 2050. This demographic phenomenon change will generate socio-economics and political challenges that will require to better understand the factors affecting subjective wellbeing in older adults. In this study we aim at exploring which variables affect the subjective wellbeing (e.g., life satisfaction or happiness) of older adults living in Siberia. More precisely we interviewed older adults living in Tomsk Region. This region has a population of about 1 million people, and twelve per cent of them (approximately 50.000 people) are older adults. Little research has been conducted on subjective wellbeing of Siberian older adults. Therefore, this study provides original and new data concerning the quality of life of these older adults.

Subjective wellbeing reflect the psychological aspect of the global experience of one’s life. For older adults, a high level of subjective wellbeing has been associated with successful ageing, and thus with many positive outcomes, like for example good health and being economically self-sufficient. In this study we investigated two important components of subjective wellbeing: life satisfaction and happiness. Life satisfaction refers to the cognitive-judgmental aspects of subjective wellbeing; whereas happiness refers to the affective and emotional aspects of this construct. These two components measure closely related but distinct aspects of subjective wellbeing and thus can provide an evaluation of which factors affect overall quality of life from two different points of view, a cognitive evaluation of respondents’ situation and a description of their feelings.

Life satisfaction and happiness are associated with a large number of socio-demographic factors. In this survey, we included questions related on the factors that, according to the literature, showed to have a strong impact on subjective wellbeing. Therefore, the following factors have been included in our survey: social support (e.g., provide or receive help from people they are close to), social activities (e.g., taking care of grandchildren), emotional support (i.e., feeling appreciated by close people), self-reported health, economical situation, age, gender, marital status, education level, and the place of living. In the analyses these factors have been used as possible predictors of life satisfaction and happiness.

In this study we administered a questionnaire to older adults living in Tomsk Region. The aim was to identify the factors affecting their subjective wellbeing (i.e., life satisfaction and happiness). Life satisfaction and happiness have been considered as independent constructs and analyzed in two separated logistic regressions. A second questionnaire will be administered in June/July 2016. This second questionnaire aims to further investigate some aspect that showed to be significantly related with subjective wellbeing in the first questionnaire.

METHODS AND MATERIAL

Respondents and Procedure

A cross-sectional study was conducted in Tomsk Region (Siberian Federal District, Russia). We administered a questionnaire through face-to-face interviews conducted in respondents' homes. Six hundred respondents were randomly recruited through quota sampling. All respondents were aged 65 years or over. In each family unit, only one older adult was interviewed. All interviews were conducted in Russian by mother-tongue interviewers. Each interview lasted 40-60 minutes. Verbal informed consent was obtained from all respondents prior to the interview. Each respondent received a standard set of gift (e.g., tea, chocolate, etc.) for the participation.

The questionnaire was carried out between August and September 2015 by an organization with experience in survey research. The questionnaire included 99 items aimed at investigating difference aspect of older adults' life. To investigate which factors are associated with life satisfaction and happiness in our sample, we selected a sub-set of these questions. More precisely, we selected the questions relating to social aspects and demographic characteristics.

Of the 600 questionnaires, 111 had missing responses on one or more variable of interest, and thus were excluded from the analysis. Therefore, the final sample included 489 respondents.

A second questionnaire will be carried out in June/July 2016. The methodology and the procedure will be the same as for the first questionnaire. A new sample of 850 respondents living in Tomsk will be interviewed.

Measurements

Some of the questions were originally in English. These questions have been translated into Russian using the standard method of back-translation. Two separated logistic regression have been performed, with the following two dependent variables: Life satisfaction and happiness.

The predictors (i.e., independent variable) were questions that investigated the following factors: Caring for your children and grandchildren, receiving and providing social support, emotional support, self-rated health, satisfaction with standard of living, age, gender, marital status, educational level, and residence area.

Similar analyses will be performed on the second questionnaire.

RESULTS

The mean age of respondents was 74.4 year (SD=6.9), with 324 women and 165 men. The mean value of life satisfaction was 5.9 (SD=2.4) and the mean value of happiness was 6.2 (SD=2.1). The correlation between life satisfaction and happiness was 0.55.

Life satisfaction was significantly associated with the following factors: Self-reported health; satisfaction with standard of living; place of living; receiving help; taking care of children and grandchildren; emotional support.

Happiness was significantly associated with the following factors: Self-reported health; providing help; emotional support.

DISCUSSION

In this study we investigated which factors are related with life satisfaction and happiness, which are two important components of subjective wellbeing. Consistently with the literature, we found that different socio-demographic variables are associated with life satisfaction and happiness. Our results contribute to show that life satisfaction and happiness are similar but different components of subjective wellbeing. In fact, the predictors of these two components only partially overlap, and thus it is useful to measure both these components to have a global view of subjective wellbeing.

The follow-up questionnaire, that we will administered in June/July 2016, will provide further evidence on the factors affecting subjective wellbeing. In this second questionnaires life satisfaction and other factors will be measured by means of Likert scales. This will provide a more precise measure of subjective wellbeing. Moreover, we will translate and adapt to Russian language some Likert scale, which have been developed in English but not yet tested and validated in Russian language. These scale will furnish Russian researchers with new measures useful to study subjective wellbeing and to compare the results with those of other countries.

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Student migration from Cental Asia to Russia: the case of Tomsk

ABSTRACT

Tomsk is – one of the leading scientific and educational centers of Russia, which attracts international foreign youth and that, is what makes of consideration the study of student migration from the Central Asia republics of Kazakhstan and Kyrgyzstan to the city relevant. It is also of relevance due to the fact that students from these Republics take leading positions among foreign students. Youth represents a mobile group of migrants that can easily adapt to to the host society and yet communicate with home society which is, in our opinion, indicative of "transmigration" taking place.

KEYWORDS

Central Asia, student migration, transmigration.

ACKNOWLEDGEMENTS

Research work carried out in the framework of the project "Man in a Changing World. Identity and Social Adaptation: Past and Present" is funded by the Russian Government (grant #14.B25.31.0009).

SUMMARY

Studying student migration can ensure a broad understanding of various processes and mechanisms associated with it such as support for and interaction with international students, study programmes of interest to these students and learning process, economic benefits from student migration for the state, strategies of adaptation and integration of migrant students which is closely connected with the host society's demographic issues.

For the first time, the notion of 'educational migration', which is largely a synonym of the term 'student migration', has been introduced at a state level in the Concept of Russian Federation Migration Policy Development until 2025. It should be noted, though, that these two terms do differ to a degree. According to the typology of migration developed by L.L. Rybakovskiy, which is based on specific characteristics such as geography, structure, period of stay and purposes, 'educational migration' is different from 'student migration' in the sense that it is a broader term used for migration for educational purposes in general including – apart from undergraduate and graduate students – postgraduate students (doctoral students), post-doctoral researchers, and visitors for other educational purposes. In turn, 'student migration' is used to denote a migration flow that emerges based on the preconditions created for students willing to get a bachelor, master, or specialist degree in a given country.

In legal terms, student migration is regulated, with no mention of that particular term, however, by a number of legislative documents, namely 'On the terms of entry to and departure from the Russian Federation', 'On the legal status of foreign citizens in the Russian Federation', and 'On citizenship of the Russian Federation'.

The processes referred to above have by now been quite well studied. Worth noting in this regard are works by L.L. Rybakovskiy, A.L. Arefiev, F.E. Sheregi, G.S. Vitkovskaya, A.P. Katrovskiy, L.I. Ledenyov, E.V. Tyuryukanova, D.V. Poletaev, S.V. Dementieva, etc. Along with quantitative methods, which most modern research builds upon, qualitative methods used chiefly in socio-anthropological research are believed to be of much importance as well. Qualitative methods, for example, were used by analyst of the Centre for Institutional Research at Higher School of Economics (Moscow) D.S. Drozhzhina in a case study of international students of Tomsk. We agree with the key methodological point made by her, namely 'it is important to get an idea of how adaptation process is developing rather than to get a result indicative of a certain moment in time'.

Having analyzed the body of work mentioned above, we came to a conclusion that no one of the authors, apart from B.I. Rakisheva and D.V. Poletaev, has studied migrant students coming from Kyrgyzstan and Kazakhstan as a separate category

of migrants. Thus, our objective was to look at student migration from these two countries to Tomsk, with a particular emphasis on communities of Kazakh and Kyrgyz students as a part of the city space, namely to study their adaptation practices and self-identification.

The city of Tomsk is one of the largest centres of science and education in Russia. It attracts a lot of international students from the CIS (Kazakhstan and Kyrgyzstan) and other countries of the world which makes it a unique 'field' for researching student migration.

The anthropology and sociology of migration tend to pay greater attention to labour migration whereas Russian researchers study student migration largely with regard to secondary education which is, again, associated with research on labour migration where labour migrants' children are in focus but from a slightly different perspective. Yet, there has recently been a proliferation of theories dealing with intensely globalized realities and of the notion of transnationalism aiming to bridge the gap between 'Us' and 'Them' which are of great interest in the context of our research.

Our view is that student migration in higher education, with all the specificities of this kind of migration due to regional and local contexts of the two countries under study and the city of Tomsk, and cultural characteristics of migrants themselves – all taken into account, constitutes a phenomenon which can be studied through the lens of transnationalism. We believe that the two concepts mentioned above are comparable and in many respects equivalent and this is what we tried to reflect in our work. We, thus, drew on the body of literature on transnationalism studied within the anthropology of migration.

It is noteworthy that Nina Glick Schiller's theoretical framework for 'transnationalism' as a mobile category with 'flexible' adaptation background has not been applied to studying student migration before and, in our view, it is of great interest with regard to studying migrant students from an anthropological perspective.

Moreover, the very term 'migration' needs to be looked at. The International Organization for Migration Glossary defines migration as "the movement of a person or a group of persons, either across an international border, or within a State... for different purposes". Student migration from the already independent republics, undoubtedly, meets the 'conventional' criteria of migration set in the study of this phenomenon. Many people can be called migrants whereas student migration involves a specific group of migrants. Thus, one could assume that student migration outside the context of communities which create a certain discourse about it does not exist. And if we erase all the boundaries and frames concerning student migration, migrant students themselves as a community will cease to exist. However, we know that every year flows of students enter Russia from the CIS countries to study at Russian universities. It is for this reason, as was found out earlier, that among international students from Kazakhstan and Kyrgyzstan in Tomsk there are those who do not identify themselves with migrant students at the levels at which they are defined as such by academia or the host society's legislation. This has driven us into looking at these people through the prism of transnationalism.

Apart from sources and literature, of great importance for an anthropological study is empirical, field material itself. Over the last two years, from 2014 to 2016, there was fieldwork carried out by us in the Republic of Kazakhstan which included collection of information in the form of expert interviews, interviews with prospective students who had been planning to study at Tomsk, and of some relevant photo materials. In parallel, the fieldwork was being done in the city of Tomsk where a number of interviews were taken with students from Kazakhstan and Kyrgyzstan studying at Tomsk and with graduates of Tomsk universities who after graduation have stayed in the city, as well as with employees at organizations responsible for registering foreign citizens at the place of stay in Russia and with representatives of university divisions dealing with international students. There were also expert interviews taken with the leaders of Tomsk national-cultural organization 'Kyrgyzstan' for a multifaceted analysis of factors of identity transformation in students from different ethnic backgrounds through transnational networks. We also collected material in the form of thematic structured interviews with Kyrgyz students. To search for possible transnational networks, 100 social media 'VKontakte' accounts of migrant students were analyzed. Apart from interviewing, in the first half of 2015 fieldwork was carried out at student dormitories in Tomsk focused on the phenomenon of student parcel and building of migrant students' community, drawing on the Actor-Network Theory (ANT).

As a result, we concluded that CIS students, namely from Kazakhstan and Kyrgyzstan, that study at Tomsk constitute 'transnational' communities which form networks of students – 'transmigrants'. This approach allows analyze the 'new' type of migrants that encapsulates life motivations, values and rules of behaviour received from both the host and home countries without being assimilated in the recipient society or losing connection to the donor society which is facilitated by modern technology development and the Internet and which can be applied in the study of adaptation and integration processes among international students of Tomsk through the prism of transnational networks.

ADDITIONAL INFORMATION

With Anton Sadyrin.

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Active ageing index: russian study

SCIENTIFIC ORGANIZATION

National Research Tomsk Polytechnic University

ABSTRACT

There are a lot of different indicators that show economic, social and human progress and wellbeing of older people. But the studies often do not allow to compare the Russian data and results with data and results from other countries because of the differences in methodology. At this study we collect the data on the basis of Active Ageing Index methodology in Russia. We have calculated the AAI indicators at national and subnational level. It was found that total AAI for Russia accounts for 30,2 points, which corresponds to 22nd rank among 29 countries (European Union and Russia).

KEYWORDS

Active Ageing Index, wellbeing, older people, Russia.

ACKNOWLEDGEMENTS

This work was performed by the authors in collaboration with Tomsk Polytechnic University within the project in Evaluation and enhancement of social, economic and emotional wellbeing of older adults under the Agreement No.14.Z50.31.0029. Moscow. The main ideas of this study were presented at International Seminar "Building an evidence base for active ageing policies: Active Ageing Index and its potential" (Brussels, 16–17 April 2015).

INTRODUCTION:

Demographic changes of past century have caused changes in population structure and as the result there is a sustainable tendency of increasing share of older people. Third and fourth age adults can be described as people with some features, first of all high level of morbidity and mortality, low level of mental health and physical activity. They often need help with routine daily activities. They often feel themselves lonely and helpless. They are very upset because of exclusion and they want to take part in society. These are the main reason for investigation how in can be possible to change the meaning of old age in modern society, solve the ageism problem, enhance active ageing, improve wellbeing of older people.

WHO suggests the following definition: "Active ageing is the process of optimizing opportunities for health, participation and security in order to enhance quality of life as people age" (WHO, 2002). The main goal of active ageing is "to extend healthy life expectancy and quality of life for ALL people even they are frail, disabled or need of care". There are a lot of determinants of active ageing which are similar to national wellbeing measurement: health and social services, behavior, natural environment, social environment, economy, personal attitudes. In this regard we can conclude active ageing concept and wellbeing concept are very close to each other but not identical.

METHOD:

For study and measure active ageing across the world Active Ageing Index (AAI) was developed. In European Union the 2012 year was the European Year for Active Ageing and Solidarity between Generations. AAI defines active ageing as "the situation where people continue to participate in the formal labor market as well as engage in other unpaid productive activities such as care provision to family members and volunteering and live healthy, independent and secure lives as they age" (Active Ageing Index, 2012). But methodology of AAI consists of indicators which can be measured on the basis of European Union statistics and it is necessary to develop cross-cultural research to study differences in active ageing across the world. We have studied AAI domains in Russia and at subnational level of Russian Federal Districts to find methodological and real life challenges in the process of evaluating and enhancing wellbeing of old adults in Russia.

There are some data resources which are available to study active ageing and to evaluate Active Ageing Index for Russia. We use AAI methodology and AAI data about completed studies (28 countries), data from Federal State Statistics Service - FSSS (Russia), from European Social Survey (6-2012), Generations and Gender Survey (GGS) Russia Wave 1 (2010). For most of indicators we used data from ESS and GGS because lack of information about active ageing in other global and national databases.

RESULTS:

Our research showed that total AAI for Russia accounts for 30,2 points, which corresponds to 22nd rank among 29 countries. Considering the contribution of each domain in total AAI it is possible to resume that independent and secure living (41%) and capacity and enabling environment for active aging (34%) are the most contributing domains.

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Identifying Social Anthropology Within the Russian University System: the case of Tomsk

ABSTRACT

Based on the example of how social and anthropological research is organized at Tomsk State University, the authors discuss main problems of the discipline's current identification within the Russian university system. The necessity is shown of changing the widespread paradigm in the positioning of social anthropology in the domestic system of academic-educational coordinates and of inclusion of it in the sphere of social sciences.

KEYWORDS

Ethnology, socio-cultural anthropology, contemporary problems of anthropology, academic journals, university education, field studies, international experience.

ACKNOWLEDGEMENTS

The presented results were produced within the framework of the project "Man in a Changing World. Identity and Social Adaptation: Past and Present" (the RF Government grant No. 14.B25.31.0009).

SUMMARY

The discussion of issues in and prospects of the development of anthropological research in Russia is conducted more or less actively starting from the institutionalization of this discipline in the academic space of our country, primarily as ethnography, then ethnology, then as one of the additional history discipline then again as ethnology and in the last 20-25 years more often as social/cultural, social and cultural anthropology or simply as anthropology. The most widespread problems

of the discipline's current development are parochialism or rather habitualness of thematic boundaries of the research, poor representation in higher education institutions and considerable distinction of domestic university anthropology from the models that have been practiced for decades in the world educational space, the deficiency of high-quality textbooks, and almost a complete lack of high-quality professional journals in the Russian language publishing works on different fields of anthropological knowledge and others [1].

The situation is growing increasingly complex due to self-presentation in most cases of the organizational units of (socio-) anthropological orientation as historical. Departments, centers, laboratories of ethnology, ethnography, and social anthropology are a constituent part of faculties of history and institutions at Russian universities: such is the case for the Department of Ethnology in Lomonosov Moscow State University and the Department of Ethnography and Anthropology at St. Petersburg State University with profession-oriented structured units in the universities of Kazan, Omsk, Tomsk, Yakutsk etc. Consequently, even in the case of licensing in these universities (not many universities have it) bachelor's and master's programmes in "Anthropology and Ethnology", the training of students compulsorily was included in the curriculum of the Faculty of History and was substantially filled with historical disciplines. The only exceptions are the Academic Center of Social Anthropology at Russian State University for the Humanities with immediate subordination to the rectorate and European University at Saint Petersburg, where an independent Faculty of Anthropology is opened.

One more substantial problem, probably the most difficult to solve, is not even an impossibility to license majors or impossibility to organize qualitative academic curriculum. Both can be easily achieved: many colleagues get acquainted with the design of educational programs in the USA and Canada, Western Europe, Japan and China. Such a problem is in fact an impossibility to provide openness for competition to fill vacancies and invite educated specialists. All our colleagues face such a problem. Some of them solve it thanks to personal international connections or using the opportunities that are given by universities to invite colleagues for short-term exchange programs (Fulbright, etc.).

The example of the Laboratory for Social and Anthropological Research (LSAR) at the Faculty of History of Tomsk State University compiling our report illustrates the essential possibility (that is possibility in principle) to solve a considerable part of the above noted problems with targeted social assistance. In just three years of implementing the megaproject "Man in a Changing World. Identity and Social Adaptation: Past and Present" the educational and research landscape of TSU has changed fundamentally.

Our own laboratory was opened and its bilingual site started functioning (http://lsar.tsu.ru/ru/). At first, a four-fold structural anthropology model usually called the Boasian model was accepted which includes 1) social, cultural, or socio-cultural anthropology; 2) linguistic anthropology; 3) biological or physical anthropology and 4) archeology. The Journal of Siberian Historical Research, created thanks to the mega-grant funding, was redesigned and conceptually renewed. After two years of its existence in the updated form it has been accepted for inclusion in the Scopus international database and effectively enhanced the international profile of "Tomsk" anthropology [2].

In the 2015-2016 academic year, major educational both bachelor's and master's programmes in "Anthropology and ethnology" were launched at the Faculty of History [3]. Key admission figures for the 2015-2016 year equated to 10 state-funded places in bachelor's programme and 7 in master's programme whereas in 2016-2017 there were 10 and 10 places available correspondingly. Preparation for basic vocation-related subjects is fulfilled by the staff of the Faculty of History and LSAR, 16 people in total. Among them there are 5 holders of 'Doctor of Science' and 9 holders of 'Candidate of Science' (PhD) degrees. Three of them have academic degrees in "Ethnography, Ethnology and Anthropology" (specialty code 07.00.07), and one person – in "Anthropology" (specialty code 03.03.02). In general, the academic staff fully meets the requirements presented by the Federal State Educational Standards on majors 460303 and 460403. But the lack of subject specialists as well as young specialists does not allow us run the whole educational process on a high level. A solution was found through inviting on a regular basis outstanding Russian and foreign specialists to deliver lectures and seminars. In 2015-2016, besides the project manager's lectures, lectures were also delivered by E.V. Miskova (MSU), M.L.Butovskaya (Institute of Ethnology and Anthropology, RAS), E.G. Trubina (Ural Federal University, Yekaterinburg), N.V. Ssorin-Chaikov (Higher School of

Economics, Saint Petersburg), P. Finke (University of Zurich), J. O. Habek (University of Hamburg), A. Halemba (University of Warsaw), O.V. Korneev (University of Sheffield), and others. The megagrant allowed not only essentially broaden the staff and courses available but also diversify our fieldwork options and organize outside-Tomsk schools for students.

One of the most important achievements during the project implementation was the widening of the term "anthropology" and of its semantic content along with the broadening of colleagues and students' research horizons. A combination of both as it turned out was not so painless, at any rate not so trivial, as could have been suggested. The first international school in which several TSU students took part became a challenge if not a culture shock. A week in the Alpine School in Italian Valle d'Aosta required skills to search for and to find anthropological scenarios (that are completely different from those in the Siberian "ethnographical field") while being surrounded by crowds of tourists, in city cafes, confectionaries and basement beer bars, in the seemingly demonstrative "traditionalism" of the local cities and their grand symbols of the bygone epoch of ancient world and medieval times which in point of fact turned out to be part of the Valdostans' daily routine – the life that an ethnographer must be interested in when being in the "field". Further "immersions" in other "fields" went more smoothly, each time opening new unexplored facets of anthropological viewing and of participants' own research skills. The new view of the subject and object of anthropological research which eventually matured is vividly reflected in the topics of bachelor's theses where there are also topics from the fields of applied and economic anthropology, migration anthropology, the study of heterogeneous communities, civil identity and national politics, etc.

Close collaboration with specialists with background in the archeology of heritage (which is inconceivable without digital technologies today) is a great achievement of the Tomsk anthropological school. Unmanned flying vehicle, 3D scans, 3D printers, computer models spinning in the air right in front of your eyes – all these became a customary, constituent part of the work of the Laboratory for Social and Anthropological Research staff and what is more important is of the students who have the opportunity not only to participate in such projects but to basically live this atmosphere.

We agree that the resulting model of Tomsk anthropology might be defined (using the computer design terminology) as a 2D model as long as it is built on the synthesis of two elements: social anthropology and archeology. How soon it will become a fully-fledged 4D model including research in biological and linguistic anthropology is yet to be seen. But even now one thing is clear: the purposeful refocusing of the local ethnological school onto an internationally-recognized view of the structure and the field of modern anthropology, anthropology as one of the social sciences alone allowed us get those results that we can be proud of now. It is difficult to say whether it is the only way to break the close, long-lasting and strong connection between ethnology and history. We are ready for a dialogue with colleagues both in terms of sharing personal experience and in terms of discussing the matter with opponents who are concerned about the future of Russian science.

[1] For more detailed information see, for example: Tishkov V.A., Pivneva E.A. Ethnological and anthropological research in Russian academic science // Early Modern and Contemporary History. 2010. No 2. pp. 3–21; Sokolovskiy S.V. In a zeitnot: notes on the state of Russian anthropology// Laboratorium. Journal of Social Research. 2011. No 2. pp. 70–89; Funk D.A. Discussing the development prospects of the MSU Department of Ethnology // The Historical Journal: Research Studies. 2014. No 1. pp. 93–102; Funk D.A. On the outcomes and problems of modern transformations in ethnology/anthropology in Russia // Proceedings of the XI Russian Congress of anthropologists and ethnologists. Yekaterinburg, 2-5 July, 2015. Edited by V.A. Tishkov, A.V. Golovnyov. Russian Academy of Sciences: Institute of Ethnology and Anthropology (Moscow) and Institute of History and Archaeology (Yekaterinburg), 2015. pp. 38-44.

[2] For more detailed information see: Funk D.A. Scientometrics and evaluation of publications in social sciences and humanities // Siberian Historical Research, 2016, №1, pp. 8–26. DOI: 10.17223/2312461X/11/2

[3] Both programmes were licensed and included in the TSU license for educational activity in March 2014.

ADDITIONAL INFORMATION

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Perception and action in children with ASD

SCIENTIFIC ORGANIZATION

Uppsala University

ABSTRACT

The typical symptoms expressed by children with autism are related to deficiencies in perception and action.

KEYWORDS

Perception, action, autism, prediction, social interaction.

SUMMARY

The typical symptoms expressed by children with autism are related to deficiencies in perception and action. The ability to predict what is going to happen next is crucial for the construction of all actions and children develop these predictive abilities early in development. Children with autism, however, are deficient in the ability to foresee future events and to plan movements and movement sequences. They are also deficient in the understanding of other people's actions. This includes communicative actions. A promising neurobiological interpretation of ASD that gives explanations to both the motor impairments and the social impairment relies on the fact that long connections in the brain are underdeveloped.

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Student

Characteristics of the disturbances of attachment of children living in different social environment types

SCIENTIFIC ORGANIZATION

Saint Petersburg State University

ABSTRACT

The influence of two types of intervention on disturbances of attachment frequency and severity was studied. Structural changes and training were organized in the orphanage A, training only was provided in the orphanage B, the orphanage C received no intervention. Disturbances of attachment were assessed by using 'Disturbances of Attachment Interview'. According to the hypothesis, children from the orphanage A are supposed to show the least frequent and severe marks of disturbances of attachment, children from the orphanage C - the most, with the orphanage B in between.

KEYWORDS

Attachment, reactive attachment disorder, disinhibited social engagement disorder, restructurisation, early intervention.

ACKNOWLEDGEMENTS

This research is supported by the grant from the Government of Russian Federation №14.Z50.31.0027.

SUMMARY

The results of the research will be presented at the conference. Structural changes and training were organized in the orphanage A, training only was provided in the orphanage B, the orphanage C received no intervention. Structural changes included modifying the caregivers' schedule to increase the consistency of their participation in children's lives. Training was aimed to enhance the caregivers' sensibility and responsibility to child signals. According to the hypothesis, the least frequent and severe marks of disturbances of attachment are supposed to be found out in the orphanage A, where both types of interventions took place.The results of the

research will be presented at the conference. Structural changes and training were organized in the orphanage A, training only was provided in the orphanage B, the orphanage C received no intervention. Structural changes included modifying the caregivers' schedule to increase the consistency of their participation in children's lives. Training was aimed to enhance the caregivers' sensibility and responsibility to child signals. According to the hypothesis, the least frequent and severe marks of disturbances of attachment are supposed to be found out in the orphanage A, where both types of interventions took place. The orphanage C received no intervention, thus it is expected to show the poorest results. The orpahage B, where only one type of intervention took place, is likely to be in between.

Ivanova Vera

PhD

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SCIENTIFIC ORGANIZATION

Higher School of Economics

Grain prices in the Russian Empire: did convergence come by train?

ABSTRACT

The paper studies the behavior of grain prices in the Russian Empire in the period from 1860 to 1913. Using annual historical data, I study 1) the impact of spatial relations between regions on regional disparities in grain prices; 2) the impact of railway network on price differences between regions. I show that the data on prices in provincial cities of the Russian Empire yield strong empirical support for convergence in grain prices across gubernias during the period under consideration. I find that the effect of railways on grain price convergence was significant, but rather small.

KEYWORDS

Railways, grain, price, convergence, Russian Empire.

ACKNOWLEDGEMENTS

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SUMMARY

This paper studies the behavior of grain prices in the Russian Empire in the period from 1860 to 1913. Using annual historical data, I study 1) the impact of spatial relations between regions on regional disparities in grain prices; 2) the impact of railway network on price differences between regions. I show that the data on prices in provincial cities of the Russian Empire yield strong empirical support for convergence in grain prices across gubernias (regional units) during the period under consideration. Spatial autocorrelation analysis points to the need for taking into account the role of proximity in regional price convergence. Finally, using data on railroads commissioning, I find that the effect of railways on grain price convergence was significant, but rather small. I argue that the effect of railways on price gap reduction increased with the time passed after a pair of gubernias had linked by railroads.

Kashapova Elmira
PhD student

Social Desirability Bias of Participants of a Financial Pyramid and its Influence on an Individual's Well-being

SCIENTIFIC ORGANIZATION

National Research Tomsk Polytechnic University

ABSTRACT

The paper considers characteristics of a man's financial behavior resulting from demographic changes and transformation of the market of financial services, where hierarchical structures, resembling financial pyramids, emerge. Citizens of Tomsk and Tomsk region were polled to reveal essential characteristics of decision-making about joining financial pyramids. A hypothesis about social desirability of considering a financial pyramid as an element of the market of financial services was tested.

KEYWORDS

Financial behavior, financial pyramid, social desirability, well-being, decision-making, senior citizens.

ACKNOWLEDGEMENTS

This work was performed by the author in collaboration with Tomsk Polytechnic University within the project in Evaluation and enhancement of social, economic and emotional wellbeing of older adults under the Agreement No.14.Z50.31.0029.

INTRODUCTION

Man's well-being is considered in terms of four key domains: material wealth, social environment, education and employment, physical and psychological well-being (man's health) [1]. Man's financial situation is greatly conditioned by his financial behavior. People's financial behavior is one of the most important indicators of social and economic well-being. It is directly linked to investment activities and redistribution of monetary resources and is exhibited in different types of financial activity: savings, insurance, consumption, credit financing, profit accumulation (including as it relates to pension formation) [2]. Man's financial behavior, in its turn, is influenced, on the one hand, by parameter variations of the market of financial services: expanding the assortment of financial products, increased number of organizations offering them, complicated consumption of financial products due to implementation of informational technologies. It allowed keeping down the costs of financial products implementation, though, complicated the process of their consumption for those who do not have technical expertise and consider information technologies to be too complex (e.g., retirees). Meanwhile, combative advertising of financial services boosts consumption of financial products which might be of no use to people.

On the other hand, man's financial behavior is influenced by socioeconomic and demographic changes: ageing of population; increase of personal disposable income of population, which expands opportunities for consuming financial services; increase of dependency ratio. Tomsk region also experiences an increase in the dependency ratio measuring the burden of retirees on working-age population.

Cost planning is the basis of financial security at any age, especially at pension qualification age, because after retiring man's income usually reduces. Though the average granted pension in Tomsk region has increased in recent years (in 2013 – 10982 rubles as compared to 2781, 6 rubles in 2005), it amounts to only 38, 1% of the average gross payroll [3]. Therefore, senior citizens have to save part of their income for a rainy day, practicing self-denial.

To maintain the same consumption level many retirees keep working after retiring. For instance, about 40% of retirees in Tomsk region keep working, as confirmed by the sociological polls data held in Tomsk region under the project plan. The poll found that the primary source of revenue for senior citizens in Tomsk region in the order of decreasing is: pension, salary and social securities. Retirees could get an extra revenue in the form of savings (bank deposits), rental income from renting out real properties, supplementary pension from non-state pension funds [4].

In an attempt to improve his material wealth a man can fall the victim of a financial pyramid. In our research a financial pyramid is an organization which attracts

participants' (investors') payments promising high interest rate, and which pays dividends to participants from the money of new members [5].

Three major approaches can be distinguished to explain people's participation in financial pyramids: economical, sociological and psychological [6].

The economical approach explains people's participation in financial pyramids by information asymmetry, i.e., people are unaware of the progress of investment projects, because organizers do not provide exact information of their activity.

Sociological approach means influence of mass media on people, creation of a total infatuation effect, an effect of a crowd. Sociologists also view trust as a factor of a mass investment behavior [7].

Psychological approach is grounded on people's inclination to make mistakes, which can result in people's participation in a financial pyramid.

In this article we will consider the influence of psychological characteristics on making economic decisions concerning income distribution and investing in projects of the kind.

The aim is to identify interrelation between man's behavioral mistakes, his decision to join a financial pyramid and its influence on people's well-being.

Next issues must be solved to achieve the object:

- to determine peculiarities of a man's financial behavior and his well-being, including senior citizens;

- to hold an opinion poll among citizens of Tomsk and Tomsk region to determine social signals of participation in financial pyramids which negatively affect man's and society well-being;

- to test a hypothesis on existence of social desirability among participants of a financial pyramid.

METHODS AND MATERIALS

Participants of financial pyramids often assume such schemes as real projects, e.g., promotion of business ideas, a social project or a benefit association. Psychologists and specialists in behavioral economics call this effect a social desirability – an inclination to exhibit socially-desirable characteristics and conceal undesirable ones [8]. People who lost money in a financial pyramid conceal the fact of their participation.

Thus, in the paper a hypothesis was made that participants attribute socially-desirable characteristics to financial pyramids. In other words, a financial pyramid allows its participants manifesting socially-desirable signals: when they consider a financial pyramid to be a charitable project, they are ready to invest, since they expect some help in return; in case of promoting a business-idea, they expect their business to be developed; in case of a social project they are part of a social group.

The hypothesis was tested through analysis of the polling data, held in Tomsk and Tomsk region. An electronic and face-to-face polling were held. People participating in financial pyramids were polled. To understand participants' behavior people not participating in financial pyramids were polled too. The poll sampled 200 respondents and had 59, 8% of women and 40,2% of men. Different age groups (18-70+) were interviewed.

Next blocks of questions were on the check-list: questions aimed at revealing effects encouraging people to join financial pyramids, appetite for risk, gambling addiction, an ability to make behavioral strategies, financial literacy; social and demographic characteristics (gender, age, education, income level, etc.); respondents' investment interests.

DESCRIPTION AND RESULTS DISCUSSION

Every man can make mistakes when taking decisions, he cannot allow for all possibilities, weigh expenses and income in all situations. His psychological and psycho-physical characteristics do not always correspond to the level of complexity of the tasks and problems under study. Mistakes, considered to be a human element, are usually unintentional. A man does wrong actions regarding them as correct or the most suitable.

Considering psychological characteristics of a man's behavior, it is difficult for a man to meet the requirements of homo economicus. In economic reality there are hardly any situations, when all participants on the market have exact information about the subject of transaction. Man's cognitive abilities are limited, moreover, his reasoning is subject to systematic bias.

People often make decisions on the basis of a working rule, not always logical one. They can make mistakes or have biases of the same kind. It can explain why most people react to the same signal (e.g., analytic's opinion) or have similar biases. Generally speaking, cognitive distortions, as a whole, can significantly influence a man's behavior in case of "social contagion" with ideas and emotions (sparked euphoria or fear), resulting in herding mentality or group thinking. These mistakes can lead to making inefficient decisions, influence prices and profit on the market. On the market, in this case, there can emerge players trying to gain from inefficiency. An attempt to attribute your actions to desirable social context is an example of social desirability bias.

The hypothesis of social desirability was tested in the following way: the key questions were grouped according to three domains:

1) Participants join a financial pyramid because other people do it;

2) Participants of financial pyramids tend to trust people, celebrities, friends, acquaintances, success stories, etc.;

3) A financial pyramid allows participants manifesting socially desirable signals.

Every domain was tested. 1) Participants join a financial pyramid because other people do it: a) people joined a project because neighbors, relatives, friends advised it or b) they were attracted by repeated advertising in mass media, street advertising, commercials on the internet (social networks); c) they told everybody about joining a financial project; d) they believed that if a friend and other participants of a financial project gained some profit, they also have a big chance to win (earn income). This condition is proved with the given algorithm (over 20% of results rating). Therefore, participants are subject to the effect of total infatuation (it is also proved in research made by Radaev V.V.), the given characteristics is an important factor.

2) Participants of financial pyramids are likely to trust other people, celebrities, friends, acquaintances, success stories, etc.): a) they joined a financial project because specialists, actors, celebrities advised it or because office environment inspired confidence; b) reliable documents were provided to participants; c) people believe that if a friend or other people gained from participation in a financial project (earned income), they also have a strong chance to win (earn income); d) they consider participants of financial pyramids to be lucky, successful, clever and calculating people. Few participants joined a financial pyramid because celebrities recommended it. However, it must be noted that financial pyramids of the 1990s became popular due to advertising and celebrities inspiring trust.

3) A financial pyramid allows participants manifesting socially-desirable signals (a charity project; promoting a business idea; a social project: a) they joined one or some projects which can be exemplified as financial pyramids; b) they considered the project to be a charitable act (a benefit association, i.e. participants expect that if they helped anybody their money would return), promoting a business idea, a social project. These characteristics, typical for participants, suggest the effect of social desirability.

Consequently, the analysis results show that participants of financial pyramids tend to attribute socially desirable characteristics to financial pyramids. This behavioral mistake encourages making a decision on joining such schemes which, thus, decreases people's well-being and shakes faith in real financial projects.

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Endogenizing monopolistic competition

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ABSTRACT

We show that a market involving a handful of large-scale firms and a myriad of small-scale businesses may give rise to different types of market structure, ranging from monopoly or oligopoly to monopolistic competition through new types of market structure. In particular, the free entry and exit of small firms incentivizes the big firms to sell their varieties at the monopolistically competitive prices.

KEYWORDS

Dominant firms, competitive fringe, monopolistic competition, contestability.

ACKNOWLEDGEMENTS

We gratefully acknowledge the financial support from the Russian Federation under the grant No 11.G34.31.0059 and the Economics Education and Research Consortium (EERC) under the grant No 08-036 and the grant 15-06-05666 from RFBR.

SUMMARY

We show that a market involving a handful of large-scale firms and a myriad of small-scale businesses may give rise to different types of market structure, ranging from monopoly or oligopoly to monopolistic competition through new types of market structure. In particular, we find condition under which the free entry and exit of small firms incentivizes the big firms to sell their varieties at the monopolistically competitive prices, as if they were to behave like multi-divisionalized firms. The structure of preferences is the main driving factor for a specific market structure to emerge as an equilibrium outcome.

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Does infrastructure mean innovations?

SCIENTIFIC ORGANIZATION

European University at St. Petersburg, Center for Science and Technology Studies

ABSTRACT

Infrastructural projects became one of the innovative policy tools of the state to develop high tech in the country. I analyze the discourse around constructions in Kazan and argue that infrastructure and buildings became a metaphor of innovations. Metaphorical nature of constructions allows various actors to impose meanings and interpretations, which explains how and why buildings became a metric to evaluate performance in innovative activity and sheds the light over urban space development and investments into new architecture in places which are meant to be high-tech hubs.

KEYWORDS

Infrastructure, high-tech hubs, Skolkovo, Innopolis, metrics of innovations, urban development, migration.

SUMMARY

Since the Medvedev's presidency in 2008-2012, innovations became a vivid part of the national discourse in Russia. It was a major initiative of former Russian President Dmitry Medvedev to modernize the Russian economy, high tech and information technologies have been a priority for federal and local authorities. High tech claimed to bring economic growth and better living for the society, make the country internationally competitive and prove the idea that Russia is one of the leading technological countries in the world.

State policies for the development of high-tech industry are central to this new focus on innovation, and they deploy several policy tools to achieve this new goal – innovative clusters, special economic zones, federal projects for tech park development, etc. Thus the state is planning to create several innovative centers across the country. Since 2007, the state has placed an emphasis on tech-parks and developed a program to support innovations and attract high-skilled migration to the region. All of these policy tools are claimed to be innovative infrastructure, which eventually will form innovative hubs around them.

In this presentation I want to focus on the notion of infrastructure – what it means for various actors, involved in the discourse around innovations and high-tech hubs establishment.

Since the very launch of tech-park program, the definition of infrastructure was not documented officially. For instance the document titled as Complex program "Establishment of Tech parks in the field of high tech in the Russian Federation", issued in 2006, does not include infrastructure in the definition of a tech park. However infrastructure means material engineering and transport communications, which are the bases for any tech park to appear and function. In this regard the concept also includes "residential" and "social" infrastructure, which legitimizes establishment of hotels, residential areas or other types of constructions.

In the document of 2011 well-developed "internal" and "external" infrastructure appears as one of the key features to justify business plan and business strategy of a Tech Park. This document requires that every tech park needs to submit factual information about the land, where the building is meant to be, such as land property, area in square meters, address, land use restrictions and encumbrances, place of tech park on the map of a city and local environment, pictures of the place etc. Other information refers to the project of construction, reconstruction or project development - description of all the objects and areas of a tech park (laboratories, training facilities, offices etc), information on their conditions and also engineering infrastructure of this project like the networks of water, gas, energy, and communications.

In 2012 there was issued the document on the Development of special economic zone at the territories of two municipal districts – Verkhneuslonskiy and Laishevskiy in the Republic of Tatarstan. Based on this document infrastructure from now on is

not limited to the material embodiment and constructions, which is “engineering” or “transport”. It also includes “social” and “innovative” developments at a territory and legitimately justifies any developmental project for these reasons, not to speak of the some “other infrastructure” mentioned in the decree. Besides, it means that to implement a project called “Innopolis” is the same as to establish all sorts of “infrastructure”. Since infrastructure was one of the pre-requisites for innovations, its usage became metaphorical.

Infrastructure and constructions became metaphors of innovations. Because “innovations” are domain in the making, and its meaning is not yet clear and stabilized, it explains how easily new buildings as something clear, tangible, measurable and mundane became a new understanding of what “IT-innovations” are.

Relations between building and innovations (buildings as presence of innovations, buildings as the evidence of investments) appeared as a reaction to the Skolkovo story. Skolkovo, launched in 2010, meant the establishment the Russian analogue of Silicon Valley in the outskirts of Moscow. The project itself was the statement that modern Russia needs to be taken into account as an international competitive player in high-tech. The very fact of constructing the new high-tech hub in Moscow was making it clear that the new Russia’s priorities are on the breakthrough technologies like telecommunications, space, biomedical technologies, IT, energy efficiency, nuclear technologies and also nanotechnology.

However this project was highly criticized, especially in media. Even though Skolkovo is not only meant to be the territory, and the brand of Skolkovo encloses several institutions, my respondents and media tend to describe Skolkovo project as a failure. The main indicator that “something went wrong with Skolkovo” is absence of constructions. Metonymic approach somehow linked together the absence of buildings with inconsistency of the products this place was meant to produce.

While Skolkovo is associated in the media discourse with the fuzzy innovations and the absence of visible results, Kazan is said to be making something real and tangible. My research was based on the data obtained in Kazan, the Republic of Tatarstan. Compared to the other regions, Tatarstan is an outstanding case of infrastructure establishment. There have been supported several initiatives, mostly in the form of new organizations and construction of new buildings. Kazan was also chosen to be one of the places to implement this federal project of tech-parks construction. As the result there were established two tech parks for the development of high tech industry – IT-parks in Kazan (2009) and Naberezhniye Chelny (2012), and industrial park “Tehnopolis Khimgrad” (2009). Later the emphasis was made on education, rather than entrepreneurship, and investments into human capital. Therefore there were established new IT-Lyceum for children (2012), Higher School of Information Technologies and Information Systems, within Kazan Federal University (2011), and the new ambitious project of Innopolis (launched in 2012), which implies new IT-university of Innopolis and developmental project for a new city.

The fact that Kazan is investing into infrastructural projects – it recently has renovated the city center, built IT-parks, tech parks and constructing Innopolis – all of this is quite “unexpected”, as one of the IT-specialists said. Building establishment became a metric of its own: buildings started to represent Kazan as “innovative city” and constructions became a new way to evaluate performance in innovative activity.

Kazan offered a different model of innovative place, enforced with brand new buildings appearing in time and according to the state’s plan. Modern architecture of new constructions was the other advantage. What interviews have shown is that buildings started to mean different things to local actors. They were the new office buildings with comfortable workspace; they were the symbol of changes in the region, the result of money invested and the image of regional politicians taking care of people and industry. New buildings put up from scratch were easy to legitimize for the local and federal government – they were persuasive to show that “something is going on”. Buildings are tangible results of activity which cannot be clearly understood and estimated in any way.

Infrastructure became a complex of meanings. Discourse analysis shows that infrastructure can be the same as engineering communications, constructions only, or constructions with certain projects for local professional community. Both the IT Park and Innopolis have been designed to create a “beautiful picture” and thus to attract specialists into the city and to keep human capital in the Republic. Both specialists and business are the audience for these projects – it symbolizes the intention of local authorities to invest, develop and support local tech industry.

New construction is powerful symbol of changes. Russia has a long history of science cities establishment – like Akademgorodok in Novosibirsk, Obninsk, Zelenograd, and others. Historical cases illustrate that each of these projects started with new architecture, which promised new modern lifestyle and new daily practices of its inhabitants. But new time offers new challenges. If during the Soviet times architects wanted to create conditions which were believed to stimulate the rise of the Soviet science, in the late 2000s the focus is shifted to the country's need to keep specialists in the country and to prevent migration by creating good accommodations in Russia.

Projects like Innopolis and IT park in Kazan are meant to prevent, or at least to decrease the level of emigration, creating the kinds of opportunities that exist abroad within the country: *mobility is good and travelling is also good but the strategy of development of the region involves attraction of staff*, as one of the experts said. Larger cities like Moscow or St Petersburg are certain to attract of the best in terms of human resources, competences and technologies. Kazan as a peripheral city has historically lacked this kind of magnetism. The way Kazan is branding itself now, however, represents an aggressive effort to compete with the capitals and to reproduce in the provinces the same conditions which exist there, and even rival those found abroad. It explains why Kazan wants to start from scratch with the new buildings, and to invite foreign architect to impose best-practices – like in the case of Innopolis and IT-parks.

To meet these expectations, Innopolis is styled as a city of the future, keeping up with the times and the latest technologies. Its furturistic orientation is what makes this project looks promising: new infrastructure brings new expectations.

Buildings and developmental projects in Kazan helped to embed technological entrepreneurship into the vision of a new lifestyle and living, which Russian regions have never offered before - primarily because entrepreneurship is the way to get into this new architecture. The other reason for tech entrepreneurship to appear in Kazan is because this new architecture is truly able to attract such talents from across the country and associate Kazan with creativity and innovation. Local infrastructure is not only meant to provide good condition for living – it also claim to bring new research facilities, university campus and new modern offices. The main purpose of all these projects is to attract the local community of all ages into technological business, assuring them that no special competence is needed to enter the field - just a bright idea and high motivation. The kind of infrastructure being built in Kazan claims to provide opportunities for just that kind of initiative: if you want to start your own tech business, IT-parks, tech zones or industrial parks are ready to support your aspirations. IT parks, both in Kazan and in Naberezhnye Chelny, are experiencing a rush of start-uppers applying for business-incubator spots in the hope of becoming the next new tech star.

Thus infrastructure assumes broader understanding of what is meant to be established - infrastructure is supportive facilities, the frame on which "innovative ecology" is destined to appear. Since infrastructure produces conditions for innovative activity and in that manner stimulates entrepreneurship, it authorized new organizations, associated with IT or innovations to claim themselves being "infrastructure". Yet, some local specialists are still skeptical; they see the difference between mere infrastructure and the promise of a new ecology it purports to offer. Despite the enthusiastic reviews, many are withholding judgments. Some computer scientists and local software developers are cautious in their evaluation of the grandiose regional scheme, and talk rather about specific research facilities, which Innopolis offers as university and the number of companies the new economic zone will be capable of attracting. As for the idea of growing and nurturing a new ecology of innovation, one of the local programmers said, *the absence of multinational IT-companies proves the inconsistency of the hype over Kazan as an IT capital that it can be in any way comparable with the Silicon Valley.*

This complex and metaphorical understanding of infrastructure has consequences on the metrics. In other words, how to estimate whether infrastructure is successful or not? Besides well-developed engineering communications and work facilities these buildings provide, managers of such tech infrastructure like to emphasize that the true purpose of these organizations is to create synergy between various actors and to establish creative ecology. This parameter goes beyond something which can be both controlled by local management and exactly estimated by federal or local government. Despite clear and tangible result like buildings, they have become substitution of innovations. However creative innovative environment requires other metrics, which are difficult to control and estimate.

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Utilising new methodology to study of child development

SCIENTIFIC ORGANIZATION

Tomsk State University and Goldsmiths, University of London

ABSTRACT

Early development and later outcomes are linked through the development of brain systems regulating emotion, attention, self-control and stress. These brain systems are governed by a dynamic interplay between nature and nurture, and influence developmental trajectories. The talk presents an overview of the cutting edge interdisciplinary methodology applied to the study of child development.

KEYWORDS

Child development, genetically informative research, GCTA, genomewide polygenic score.

ACKNOWLEDGEMENTS

Grant 11.G34.31.0043

SUMMARY

Early development and later outcomes are linked through the development of brain systems regulating emotion, attention, self-control and stress. These brain systems are governed by a dynamic interplay between nature and nurture, and influence developmental trajectories that can be further amplified through a cascade of exposures to risky vs. protective contexts. In order to gain a comprehensive picture of the causal processes in the course of development, interdisciplinary approaches are required. The talk presents an overview of the cutting edge interdisciplinary methodology applied to the study of child development. The methods include quantitative genetic, molecular genetic, and bioinformatic advances, such as the use of genomewide complex trait analysis (GCTA), genomewide polygenic scores (GPS), whole genome sequencing, epigenetic studies, research involving IVF-conceived families and other genetically informative designs.

ADDITIONAL INFORMATION

With Elena Grigorenko.

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Korean Youth Centre «Anyong» as a place of interaction for the Korean youth in the city of Tomsk

SCIENTIFIC ORGANIZATION

Tomsk State University The Faculty of The History, Social Anthropology

ABSTRACT

This article analyzes Korean Youth Centre “Anyong” in terms of place and space of the city.The main question is whether the centre is a place for interaction or a means of communication for the Korean youth. Drawing on A. Appadurai’s theory about spaces, the centre is conceptualized both as an ethnospace formed by flows of people and a mediaspace formed by mass media and the Internet. It is concluded that for its members the centre’s nature is symbolic and the centre is both a place for and a means of interaction for the youth.

KEYWORDS

Korean Youth Centre “Anyong”, Korean youth, Tomsk, ethnoscapes, mediascapes, place.

ACKNOWLEDGEMENTS

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SUMMARY

In the present-day conditions of globalization and active international contacts the communicative intensity between nations entering a different cultural area is considerably increasing, and migration flows are increasing simultaneously. This process is acccompanied by an increase in the formation of ethnic communities and an increase in the existing diasporas. Since the 1990s diasporas have been acquiring transnational community features. As noted by Russian political expert A. S. Kim modern diasporas are specific social groups whose identity is not determined by particular territorial units, the scales of their distribution make it possible to say that the phenomenon has acquired a transnational nature.

Ethnic Koreans, having a rich history of institutional formation of their status in receiving countries, can be considered a transnational diaspora. The post-Soviet space Koreans form stable global networks. Tomsk Koreans are institutionally represented by national and cultural autonomies and the Korean Youth Center ‘Anyong’. It is fair to assume that Anyong is an example of a community with developing transnational connections, subjected to the influence of global processes.

Anyong may be considered as a symbolic place of interaction for Korean youth. As demonstrated by V.S. Malakhov, a famous Russian political expert, ethnicity possesses a symbolic nature, having been described from the perspective of social constructivism as a marker of difference, as a sign, around which any differences from biological to social are organized. Any given characteristics distinguish some individuals from others (racial, anthropological, lingual or cultural) act as a symbol in relation to which social differences can be built. It is commonly known that transnationalism is the antipode of long existing binary opposition “us” – “them” that deviate from differences, including the differences organized by the symbolic nature of community. Consequently, it seems quite interesting to observe the confrontation of symbolicity organized by Korean diaspora in the city space of Tomsk with transnationalism that is vividly traced while observing the community under investigation.

Furthermore, the Korean Youth Center is a place that forms a particular space. American anthropologist, sociologist and philosopher of Indian origin Arjun Appadurai considers space in five manifestations, marking ethnoscapes, mediascapes, technospaces, financescapes and ideoscapes, where ethnoscapes refer to the migration of people across cultures and borders; mediascapes deal with mass media and the Internet; correspondingly technologies form – technospaces; the money flow – financescapes; and ideoscapes center on the ideologies of a government and movements. It can be assumed that Korean youth centers are ethnoscapes formed by Korean youth, who moreover is mobile, i.e. they live in the conditions of globalization and obtain different resources for speedy communication with people around the world. Thus, it is fair to claim that apart from the ethnoscape, Anyong is able to build a mediascape, thereby representing itself to the public at large.

The empirical base of the research is primarily qualitative methods of research, which enabled the collection of extensive and representative material to elicit the specifics of Anyong’s development. In the course of the research the method of participant observation was used, which allowed us not only observe but also participate in events held by the Korean Youth Center that were described using the thick description method. Moreover, semi-structured interviews were conducted with the leaders of Anyong and the Chair of the National Cultural Autonomy of Koreans.

So, what acts as symbols for Korean youth in Russia? V. S. Malakhov notes that if we look at ethnicity in the symbolic production, we can identify two levels – discursive and non-discursive (corporeal). If we divide symbolic space into levels, then from the discursive point of view this level is mostly determined as “collective memory”. This, in turn, is a metaphor, therefore it is impossible to speak about the objectivity of such a marker of symbolicity. V. S. Malakhov notes the decisive role of the political elite, mass media, education and intellectuals. It is true that many Korean intellectuals, being involved in the study of the history and culture of their people, form various and even contradictory points of view regarding Korean history and its different interpretations, which cannot but influence the formation

of a collective historical memory. Furthermore, the present generation knows the history of their people from their ancestors' stories. Opinions are constructed and an overall picture is created. This might indeed be called a "collective memory", if we accept that each ethnic Korean knows the history of his/her family to a certain degree. Anyong works as a place where youth can exchange their family histories, creating a unified narrative of their people from stories.

When interpreting symbolic nature through the corporeal level, an important role is played by visual, audio and tactile images, i.e. often dances, national music, clothing and language features, etc. are factors that form group belonging. The preservation of symbolic space in the form of observing certain traditions such as celebrating the first year of life, sixty years of age and the New Year, and holding informal meetings may provide evidence that the cultural markers reflect the desire to "be Korean" – to shown one's "Koreanness". Moreover, attention must be paid to ethnic signs that can act as symbols. Thus, writing acts as a symbol. The majority of ethnic Koreans no longer speak their native language, but nowadays there is a spark of interest in its study; those who know Korean have opened language schools and offer courses that are in demand. Language courses are offered at Anyong. It is interesting that many learners on such courses are not Korean. The fact that they have to come to the center to study Korean demonstrates respect for the Korean culture and language. In turn, the center demonstrates openness and interest in its own culture and the popularization of it.

Yet another symbol is clothing. Of course, ethnic Koreans have long since started wearing European clothing. But all the official celebrations held by Anyong are accompanied by demonstrations of national costumes. Thus, during the Day of Korean Culture in 2015 visitors were able to try on the hanbok (a Korean traditional national costume) and have their photo taken.

Names as a symbol. In our case, this means Korean surnames. Despite the fact that Koreans have been living in Russia for over 150 years, Korean surnames are an important marker of Koreanness. Moreover, first names vary – they are mostly Russian, but also Kazakh or Kyrgyz, which is reflective of another symbolic nature – belonging to another culture. Therefore, in our case, we can speak about symbolic syncretism, which appears not only in formal things, but also influences identity: "I'm connected with Korean culture only by my surname and eye shape"; "When I say 'Korean Russians', I mean our mentality is completely Russian, but our blood is Korean, and nothing can change that."

Project activity. Korean holidays (New Year, First Year Celebration, Sixty Years Celebration) playing traditional instruments (samulnori), informal meetings and traditional cuisine are the symbols of "Koreanness". Anyong acts a guiding organization. Its primary function is the presentation of Korean culture, to represent "Koreanness" as cultural identity. The issue of how important and necessary it is for Korean youth requires further observation and investigation. Now it is fair to state that there is a decrease of interest and need among Koreans to manifest their ethnicity. Other values are in the forefront. Anyong acts as a public organization, uniting youth according for different reasons, where interest in the Korean culture is one of the most important, but not the only factor of unity.

Many researchers consider that the majority of transnational diasporas are formed by emigrant communities that are very mobile today preserving connections with their own country and at the same time successfully adapt to the new conditions of host society and country. At first sight the Korean diaspora of Tomsk is in a league of its own in this situation, which is transparent because today the migrant flow of Koreans from South and moreover North Korea does not amount to many people, almost none. Nevertheless, we can observe migrants, mostly migrant students from the CIS countries who having found themselves in a new community feel a need to consolidate with "the same as me". Moreover, growing connections with South Korea and a constant circulation of people can be considered as the creation of a global network, a unified ethnoscape. The Korean diaspora rises to a new level, the transnationality level. As academician V. A. Tishkov postulates, "Modern diasporas forfeit an obligatory link to a particular locality – country of origin – and gain on the consciousness and behavioral level a referential connection with particular worldwide historical and cultural systems and political powers. The obligation to one's "historical homeland" leaves the diaspora discourse. The connection is constructed with such global metaphors as 'Africa', 'China' and 'Islam'.

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Professor of the University of Paris I Panthéon Sorbonne and scientific leader of a megagrant project (URFU, Ekaterinburg)

Russian elites and European norms, models and innovations, 1700-1917: some lessons from the past in a long term perspective

SCIENTIFIC ORGANIZATION

University of Paris I and Ural Federal University named after the first President of Russia B. N. Yeltsin

ABSTRACT

The contribution will begin by a short presentation of the megagrant project, the way we conducted our works, our method and our sources. Then to explore the extreme variety of relations that took place between Russian and European elites from 1700 to 1917, the paper will focus on a few concrete examples and will rely on the concepts of circulation, diffusion and appropriation.

KEYWORDS

History, Russia Europe, international relations, elites, influence, interactions, models.

Mershieva Alena
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Techniques of active learning

SCIENTIFIC ORGANIZATION

Novosibirsk state pedagogical University, IPMIP

ABSTRACT

The study of the influence of relationships within the team to achieve a common goal and progress.

KEYWORDS

Pedagogy, teambuilding, creating an effective teambuilding techniques, temporary teams.

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Game-Theoretic Models of Social Network Formation

SCIENTIFIC ORGANIZATION

New Economic School; Moscow Institute of Physics and Technology

ABSTRACT

Empirical studies show several laws that social networks do obey and other complex networks, i.e., biological or technological do not. These laws include small diameters (“six degrees of separation”), scale-freeness (power law degree distribution) and high clustering coefficient. To find microscopic foundations to these macroscopic effects is a great and unsolved challenge. In the talk we will survey existing models an discuss how to expand them for better parameters calibration.

KEYWORDS

Social network formation, game-theoretic models. scale-free networks, clustering coefficient.

ADDITIONAL INFORMATION

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Holistic System Approach to Assess the Older Generation's Well-Being in Russia: the Need for the Russian Elderly Well-Being Index

SCIENTIFIC ORGANIZATION

National Research Tomsk Polytechnic University

ABSTRACT

This paper focuses on the development of a holistic approach to older adults' well-being evaluation on the basis of system analysis. The authors draw on the causes of interest for comparative assessment methodologies of the well-being of elderly generation. As assessment tools joining a set of objective and subjective indicators in one evaluation scale, composite indices are researched as comparative analysis methods. The paper formulates the principles of the Russian Elderly Well-being Index and analyses the possible domains for the elderly population well-being assessment.

KEYWORDS

Elderly population, well-being, objective indicators, subjective assessment, system analysis, composite indices.

ACKNOWLEDGEMENTS

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SUMMARY

The demographic shift in the population structure, associated with the increase in the proportion of the older ages, has a very serious impact on the lives of individuals, communities and the entire country. There is a necessity to develop and practically implement new tools and mechanisms for the integrated assessment of the main aspects of the elderly generation economic and social well-being.

For example, the Tomsk region at the beginning of 2014 accounts 224400 people over retirement age (men - 60 years and older, women - 55 years and older). Compared to 2011, the number of older adults increased by 17800 (or 8.6% increase) since the generation of 50s began to reach retirement age. During this period, the share of the older retired generation in total population of the Tomsk region increased from 19.7% to 21.0%. The population of the Tomsk region, according to international criteria, is considered to be "old" since the number of the people 65+ years is higher than 7% of the total population. In the beginning of 2014 this figure was 11% (every ninth resident). Also, the aging of the population is evidenced by the increase in the average age of citizens. Over the past three years, the average age of the population increased by one year from 37 years to 38 years.

In general, there are several trends in evaluating the well-being of the elderly population at the macro level:

Development of composite indices as a universal tool for cross-country comparisons in order to solve a whole range of socio-economic and political problems;

Combination of objective statistical indicators and subjective assessments in a single measurement scale that characterizes the well-being of the elderly population as a phenomenon that requires a multidisciplinary assessment approaches;

Development of national statistics, national indices and scales of subjective well-being of the elderly population monitoring which allows to assess, analyze, compare the results in different timelines and in different regions in order to develop relevant national social and economic policies aimed at improving the well-being of the elderly population.

Our model for assessing well-being of elderly adults rests on the following prerequisites:

1. Well-being is a combination of objective and subjective economic, social, physical and psychological criteria determined by a specific quality of life and char-

acteristics socio-cultural environment deeply rooted within economic, social, cultural subsystems of a country.

2. There are significant and important, often informal, support institutions for elderly adults such as social connections, communication, family, friends, neighborhood environment, etc.
3. Any socio-economic system requires formal procurement institutions acting through institutionalized structures which are responsible for resources allocation (governmental and public organizations, social welfare system, policies, etc).

While developing the structural model of the researched phenomenon, we used the hierarchy of functions related to the management and life procurement support or, in fact, to the livelihoods of various groups of older people (Fig.1). This approach allows researching multiple target groups and generating modifications of the model, depending on the research goals. Invariant parts of all models are functions of governance and procurement support. The governance functions are performed by such structural elements of the system as the "Government" and the "Economy", creating a balance between the desirable and the possible. The function of procurement support is performed by institutions and organizations, creating and supporting living environment for the elderly people. The variable part of the model is a social target group itself in a variety of individual characteristics, problems, needs and opportunities.

Fig. 1 Holistic model of the elderly population's well-being (Pavlova et al., 2015)

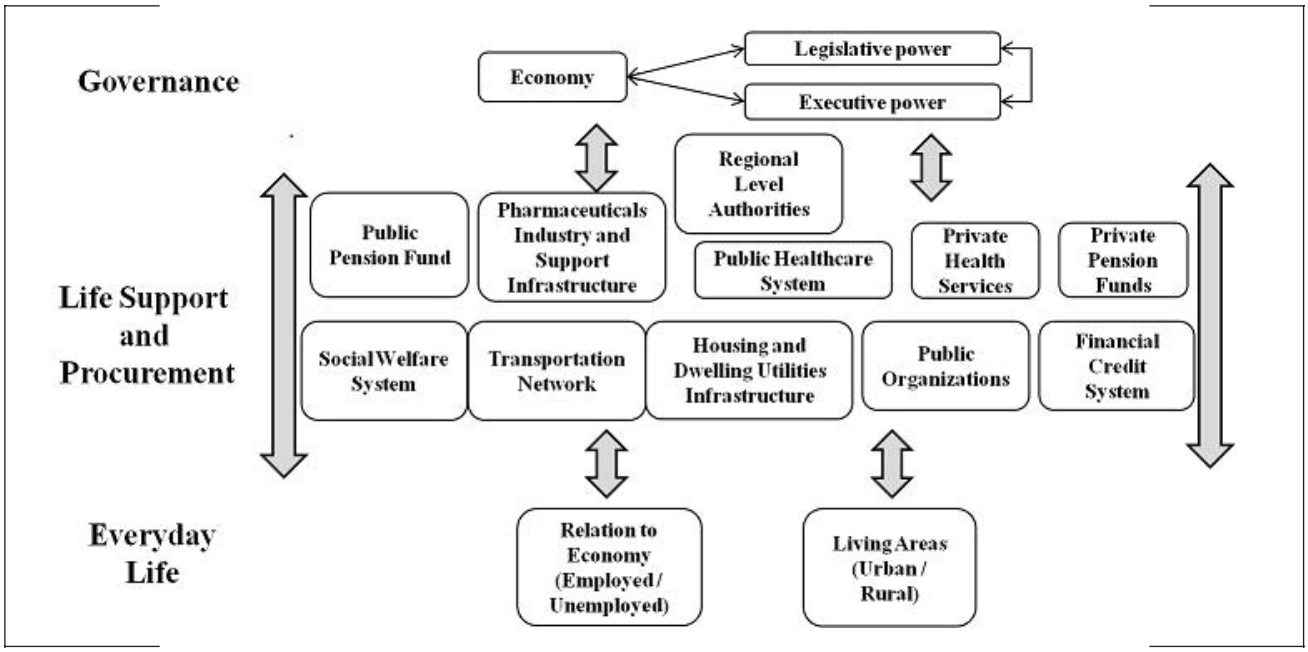
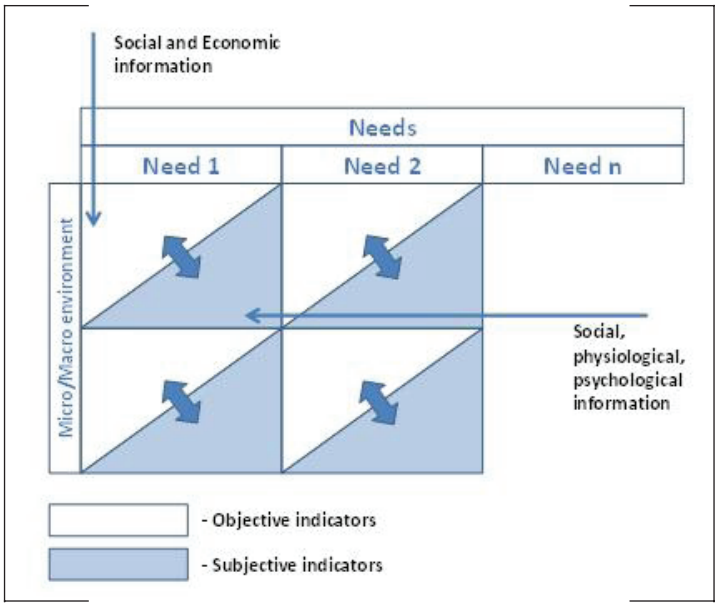


Fig. 2 Matrix of objective and subjective indicators (Pavlova et al., 2015)



We also introduced the idea of using (1) the definition of "model", (2) the concept of "identity of the model and the object" and "adequacy of the model and the object" which is applicable to any model type: structural, functional, institutional, mathematical, statistical, etc. Each model type has its advantages and disadvantages. Since they can be applied to the same object, the integrated evaluation becomes much more accurate. Fig. 2 shows a matrix of subjective assessments and objective indicators, where the columns represent a hierarchy of needs of the elderly people and lines represent scale of interactions.

As the result, the model of practical level includes the following domains of needs: (1) health and physical activities; (2) income and employment; (3) accommodation, assets and living conditions; (4) education and training; (5) social connections; (6) social activities; (7) entertainment and free time; (8) mobility. Scale of interaction is represented by institutions and organizations performing functions of procurement: (1) legislation (national and

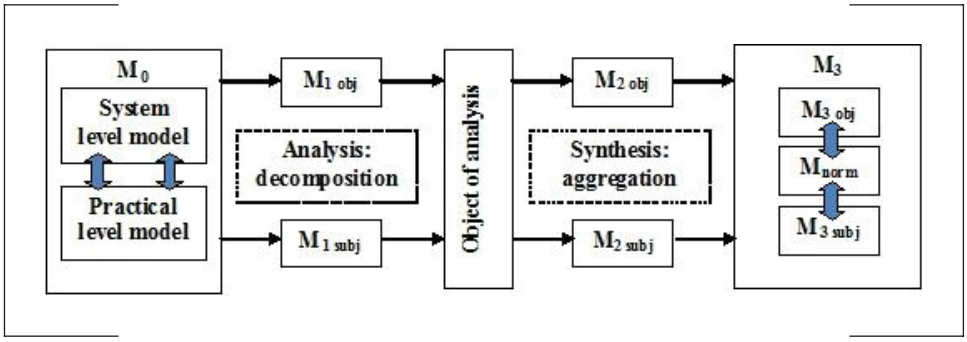


Fig. 3 Procedure of the two-level model approbation (Pavlova et al., 2015)

regional levels); (2) budget and financial government responsibilities; (3) formal government institutions of healthcare, social welfare, education and so on; (4) non-government organizations and informal institutions; (5) close social environment (friends, neighbors, acquaintances); (6) household/family (spouses; parents, children, relatives).

Evaluation of the developed model was done in several stages following the procedure presented in the Fig. 3. M0 is the initial two-level model including system and practical levels. Mobj and Msubj stand for sub-models integrating objective or subjective indicators.

As the main sources used for this study we focus on numerous databases and documents of official governmental and public authorities such as the UN, WHO, OECD, Eurostat, Russian Federal State Statistics Service (FSSS). The official statistics for Russia are withdrawn on the basis of the List of Indicators from Federal Statistical Observation Forms and the List of Indicators of the FSSS. On a special request of the authors, the information on 116 selected indicators was withdrawn by the Tomsk Regional Statistics Service (Tomskstat) which, finally, led to the release of a unique report "Evaluation and improvement of the social, economic and emotional well-being of elderly people in 2000-2013" by Tomskstat in 2015. For subjective assessments analysis we developed a survey with 78 questions resulting into 324 variables. The questionnaire was designed on the basis of the matrix of subjective and objective indicators covering 8 domain of needs and 6 functions of institutional procurement. The survey embraced 400 older adults living in the Tomsk region. At the present stage, the survey enters the stage of information synthesis and aggregation.

For this study, there are two normative models (Mnorm) selected – the Global Age Watch Index (AW) and the Active Ageing Index (AAI). Both indices the AW and the AAI are to serve as political tools as they focus on sustainable development of societies. The AAI is aimed at "providing a new tool for policy makers to enable them to devise evidence-informed strategies in dealing with the challenges of population ageing and its impacts on society" (Zaidi et al., 2013) in order to monitor (and compare) active aging outcomes at international, national, and subnational levels; to indicate older people's potential for a better inclusion in social and economic life as well as to advocate most appropriate policy measures. The AW is aimed at measuring and improving the quality of life and well-being of older people, indicating population challenges in order to generate evidence for policymakers in the first place. The AW demonstrates strong affiliation to pension watch as a tool to guarantee income security. The AAI represents a generally universal approach to measuring active ageing according to well-built methodology and its application to high-comparability data. At the same time, there is a strong limitation to such an index reconstruction for Russia, since the current data comparability is questioned. As a normative model, the index can be calculated for Russia, but with significant aberrations due to different data sources and necessary methodology modification. Nevertheless, the research team, which developed the AAI, stressed the flexibility of the index usage. We suppose that for the correct development of the AAI for Russia, it is necessary to introduce national statistical into the computation of this index or to develop a new methodological approach basing on existing data sources. This may be quite a challenging, but a very promising further research direction. Both these two indices represent a combination of objective indicators and subjective assessments. The Global Age Watch Index comprises 13 indicators (8 objective and 5 subjective ones). The Active Ageing Index has 22 indicators with 20 objective and 2 subjective ones.

Russia lacks overall general monitoring surveys of the older generation and ageing problems, though recently some new monitoring forms have been introduced by the FSSS for the nation-wide monitoring in the domain of older generation well-being for a limited number of objective indicators. In general, there is a very narrow scope of data collection on many indicators, comparable with those of foreign countries. Since the monitoring of the elderly population level of life is relatively

recent for Russia, it is still impossible to trace the dynamics for the most of the indicators for significantly lengthy time periods. Therefore, while testing the the systemic model (Fig. 1), within the project Evaluation and enhancement of social, economic and emotional wellbeing of older adults (the Agreement No.14.Z50.31.0029), we developed the database devoted to the assessment of the elderly population well-being. The database structure is developed according to the proposed model and includes: (1) Types of reserched objects such as Government, Procurement, Economy, Retired, Friends, etc.; (2) Needs and resources: Health and physical activity, Revenue, Accommodation, Development, Communications and social connections, Social activity, Leisure, Mobility; (3) Indicators (45 source indicators plus computed indicators); (4) Connections between objects, needs and resources, and indicators.

Web-interface of the database is the part of web-site http://statlwl.tpu.ru/. It allows to input and edit the data and to display data (the user needs to login in order to have an access to the database). As for the web-interface, we obtained a computer program registration certificate «The control program for database of indicators of well-being of older people», certificate of the Russian Federations' state registration № 2015619013, authors: Barysheva G.A., Monastyrny E.A., Spitsin V.V., Shabaldina N.V., Gumennikov I.V. Physical model of the database is shown on Figure 4.

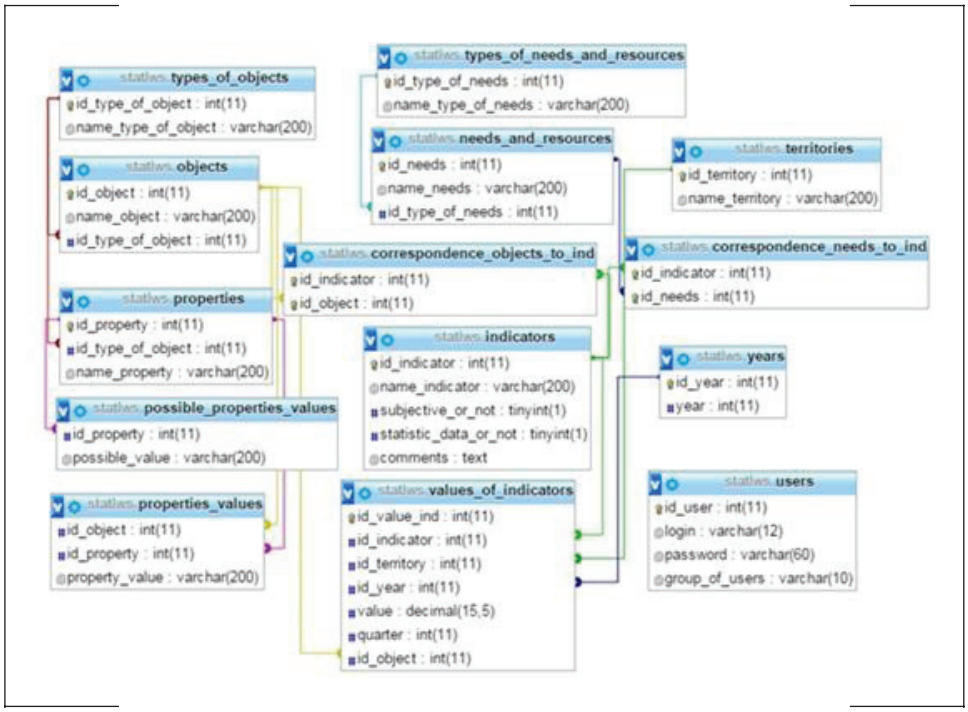


Fig. 4 Elderly population database' physical model

We consider regional social and economic comparisons in terms of their dynamics as an acute problem on the rise of a new agenda. At the time, inter-regional comparisons in Russia were mainly associated with the economic situation, basing on objective criteria. However, improving quality of life of older people is becoming one of the governmental priorities. The approaches to the statistical data collection are being reconsidered on the national level. Despite the fact, that new forms for life assessment of the older generation are introduced, this research issues bring up challenging and sensitive problems. In previous years, a comparative analysis of the elderly has been underdeveloped, so the direction for future research is a very promising comparative study of the older people well-being dynamics in different regions of the Russian Federation. Despite the fact that Russia specifically shows some dynamics in national policy on ageing, it still lacks comprehensive tools for older generation well-being measuring and analysis both on national and regional levels.

Based on the foregoing, it should be noted that the conceptual framework in creating the Russian index of the elderly population well-being should be the approach based on the needs of older generation (needs-driven approach). There are several basic principles for developing a composite index (Korchagina, 2012): data should be available and measurable, presented in official documents and regularly updated; the indicators/variables should be simple enough for interpretation and reflect the actual processes and their dynamics; the indicators/variables must be scientifically grounded and justified, be based on international standards, can be used in econometric models to measure, assess and predict development of the present situation.

In order to develop a composite index for assessing the elderly population well-being for the Russian Federation, we have formulated additional principles such as (1) possibility and necessity of heterogeneous indicators/variables aggregation in a comprehensive evaluation scale under the single methodology; (2) indicators/variables relevance implies the validity and justification of the integration into the composite index of any metric; (3) adequate, fair and reasonable allocation of weights

between variables, indicators and domains; (4) needs of the elderly population non-excludability; (5) non-excludability of territories and regions; (6) differentiation of regions and territories with the possibility of multi-level differentiation in Russia (federal districts, regions, territories) due to significant distinctions in socio-economic development levels; (7) combination and usage both the objective and subjective measures; (8) valid and fair international and inter-regional comparisons.

In addition, the research of composite indices methodologies leads to understanding the basic variables/indicators assessment groups, which are tightly connected to elderly population needs. These groups, as a rule, include the following domains: (1) health; (2) income; (3) work/employment; (4) education; (5) living conditions/ dwelling; (6) family; (7) social life; (8) political life; (9) emotional state of being/subjective perception; (10) community; (11) safety and security. Also, we can find the following areas of assessment which are more rarely used such as (1) opportunity; (2) climate/geographical conditions of living (3) gender equality and gender issues; (4) ecological conditions.

The research results allow us to select necessary domains with the relevant variables to develop the methodology for computing and developing the Russia Elderly Well-being Index (REWI) for the Russian regions. The necessity of the REWI development is justified by the current economic and political needs for the comparison of elderly population will-being for different Russian regions and territories due to the scarce elderly population well-being metrics presented in Russian statistics as well as due to significant differentiation of Russian regions in terms of demographics, income, employment, climate, dwelling specifics, etc. We intend to complete second part of the research with the analysis of subjective assessments basing on the survey conducted and compare objective and subjective criteria results. The cross-regional comparisons within the territory of the Russian Federation on the basis of holistic system approach are previewed as the next research phase.

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The Russian Elite: Values, Attitudes and Forecasts

SCIENTIFIC ORGANIZATION

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ABSTRACT

This research project analyzes the values, mindset and ideological orientation of post-Soviet elites, as well as the factors that influence their formation and evolution. Based on the results of the analysis, authors composed a portrait of a typical representative of the Russian elite in the 2020s, and forecasted how elite values and attitudes will continue to evolve and what effect they will have on the Russian domestic and foreign policy.

KEYWORDS

Russian Elite, Values, Anti-Americanism, Cohort-analysis.

SUMMARY

This study is based on empirical evidence collected from seven waves of the survey of Russian elites conducted by Prof. William Zimmerman (Zimmerman, 2002, 2009). The waves were taken in 1993, 1995, 1999, 2004, 2008, 2012 and 2016, with a total of 1,664 respondents. All respondents are residents of Moscow. Restricting the sample to Moscow is unlikely to result in statistical bias, given Moscow's disproportionate impact on the nation's decision-making. Moscow is the financial, political, intellectual, and cultural center where the principal decisions are made and the individuals occupying key positions in various spheres of public life are concentrated. To compare elite and public views (specifically, with regard to the US), the study also uses the data from the New Russian Barometer project directed by Richard Rose [Rose, 1992–2009] and administered by the Levada Center. It comprises 18 national polls conducted between 1992 and 2009. We also use some other data from the Levada Center. To analyze the value difference between the elite and mass publics, we use the data from six waves of the World Value Survey (1990, 1995, 1999, 2006, 2008, and 2011) [World Value Survey, 1981–2012].

The data provided by these polls reveal not only short-term transformations in the elite's attitudes but also some stable long-term trends involving various groups of the Russian elite. To identify generational differences in elite values, the respondents were subdivided into several generations: born in 1940 or before; between 1941 and 1950; between 1951 and 1960; between 1961 and 1970; and after 1970. The recent wave of the World Value Survey data also allows us to examine the generation born in the 1980s.

We have relied on of these data to trace the evolution of elite values and their preferences for the country's political system, economic development model, and foreign policy in the context of the Russian Federation's changing role in the international system. Based on the results of our analysis, we have composed a portrait of a typical representative of the modern Russian elite, and forecasted how elite values and attitudes (and the effect they have on the country's foreign and domestic policy priorities) will continue to evolve. Elites help shape the conceptual foundations of Russian policies and choose the means of achieving the preferred ends, but they are not always guided by rational motives in these pursuits. The influence of individual psychological traits on foreign policy decisions still has not been thoroughly studied due to the difficulty of polling officials at the highest levels of power. However, the unique data of William Zimmerman's surveys of Russian elites provide some insight.

Owing to the rigidity of psychological traits, the foreign policy preferences they inform are a good predictor of an individual's actions in specific situations. In fact, psychological traits are a better predictor of foreign policy views than group allegiance and political orientation. Therefore, the psychological component is important in any analysis or forecast of changes in elite values. For instance, ethnocentrism is an important characteristic that has been found to have an influence on foreign policy.

Some findings are counterintuitive. For instance, it would seem that a broad definition of Russia's sphere of national interest should correlate with support for defending the national interest by military means. The number of respondents supporting a broad definition of Russia's sphere of national interest (extending beyond the country's borders) has been steadily falling until the most recent wave, when the trend sharply reversed. All the while, the number of those who see military power as the decisive factor in international relations has been growing and still is. On the basis of cohort differences observed in the responses to these questions, we make several forecasts of the direction Russian foreign policy will take in the coming decades. The lowest percentage of respondents expressing support for a broad conception of Russia's national interest was found among two cohorts: those born in 1961–1970 and those born after 1971. By 2020 these two cohorts will be the largest in the Russian elite, making them especially important in any discussion of the future foreign policy.

The youngest cohort (born after 1971) were the least likely to support the use of military force as a tool of foreign policy. The growing number of elites with more aggressive views on the use of military force suggests that Russia will likely take a harder line in foreign policy matters in coming years. This will not necessarily come in the form of more armed conflicts unleashed by Russia; yet we expect more attention to all matters pertaining directly and indirectly to growing the country's military power. In this way, the elite's views on military power will shape not only the direction of foreign policy but also Russia's domestic priorities.

At the same time Russia is unlikely to use military force in the absence of any international conflict or potential threats to its national interests. For example, both respondents who broadly define the national interest and those who hold the opposite views rank economic power ahead of military power as a factor in international relations. This suggests that the elites are most likely to support using economic leverage rather than military force in peacetime.

Our forecast of the foreign policy views of the Russian elites should not be taken as a declaration of this group's expansionist intentions, though they are likely to support efforts to increase Russia's military power and to favor tougher measures, including the use of military force, in international conflicts that threaten Russia's interests. Their lack of expansionist ambitions is supported by the consistent downward trend in the number of elites who broadly define Russia's sphere of national interest. The respondents born in 1961–1970 and post-1971 are the least likely to believe that Russia's sphere of interest extends beyond its borders.

Our research also has implications for the prospects of the Russian-US relationship. The level of anti-Americanism expressed in the surveys is today considerably higher among elites and the general public than in the 1990s. Over time more respondents have come to view the United States as a threat to Russia. The most significant changes in attitudes to the US and democratic values in general were recorded in the cohort born in 1961–1970. In 1993, the majority of this generation supported democracy and liberal economic reforms, and viewed the United States as a potential partner. But in the 2000s, anti-American attitudes began to grow rapidly. This change in the attitude toward the US among these cohorts has a direct bearing on the direction of Russia's policy with respect to the US.

The rise of anti-Americanism in the Russian population is rooted in ressentiment, or disillusionment with Western values and the US as the embodiment of those values, caused by Russia's rocky transition to democracy and a liberal market economy. This hypothesis has been borne out by the data. Ressentiment explains a critical dimension of the transformation of elite values. Moreover, as our analysis shows, anti-American sentiment peaks during the periods of international tension and heightened antagonism toward a potential geopolitical rival.

Currently, the relations between the United States and Russia are turbulent, with relatively frequent disagreements on matters of international importance, like the situations in Libya, Syria, and Ukraine. Russia has not shied away from confrontation; it has dug into its positions. This could be due to the growing number of people in the 1961–1970 cohort who see the US as a serious threat to Russia's security. These are people with significant influence on Russia's foreign policy.

From this we can infer that Russia's policy to the US may undergo some changes when elites born after 1971 become more of a presence in positions that formulate foreign policy. It is entirely possible that younger elites will take a milder approach to bilateral relations and will seek out compromise. Of course, exiting the current round of confrontation would be a necessary condition for this to happen.

Our analysis of the Russian elite's perceptions of internal threats to the country suggests a number of conclusions regarding likely domestic policy priorities in the coming years. As noted above, the elites regard inefficient governance as one of the most serious threats to Russia's stability, increasing the likelihood of future efforts to reinforce Russia's vertical power system and overcome internal contradictions, as well as to stabilize interethnic relations. Ethnic strife, another major threat in the eyes of the elite, has been a source of instability in various Russian regions during the entire post-Soviet period, and has undermined efforts to strengthen the vertical power system. Still, economic problems are viewed by elites as the main source of trouble, suggesting that the main emphasis of domestic policy will be on overcoming socioeconomic challenges.

Elites are becoming more ideologically polarized over time, particularly in their political views. While the mean values on political questions are essentially the same for all cohorts, the variance can be quite different. Polarization, as measured by variance, is decreasing at the times of international crises. This re-enforces the idea that the youngest cohort of the elite may become less anti-American only if the current tension is somehow dissipated.

For the younger respondents (born after 1970), the greatest polarization is seen on questions of government ownership of industrial enterprises, the prospects for starting a new business (an indirect indicator of a respondent's positive attitudes to the market economy), the existence of a single true philosophy, and outlawing dan-

gerous ideas. The variance for this cohort was the highest for outlawing dangerous ideas, but in general this cohort is no more polarized than others, as the structure of cohort differences varies for each indicator.

The political beliefs of the Russian elite have been marked by a gradual divergence between two groups, the first of which prefers authoritarian methods of governance while the second favors a liberal democratic model. The first group is currently in the majority, but the number of supporters of liberal democracy has also grown in the past few years. Will this group exert a significant influence on Russian politics in the coming decades? That depends on a host of factors. First, will the general public support calls for liberalization and democratization? In 2011–2012, we saw an increase in protest activity due mostly to the greater political participation of the middle class. However, it appears that their energy has been dissipating, as there has not been an avalanche of new demonstrators. As noted above, international tensions seem to be a factor of consolidation. Second, much depends on cohort differences: the generation born in the 1960s will occupy key government positions in the 2010s, to be gradually replaced by those born in the 1970s in the following decade.

Rising socioeconomic prosperity in the Russian Federation could upend this course of events. If the country overcomes the ill-effects of the current crisis and economic growth continues at the same pace as in the 2000s, the elite polarization may not necessarily lead to a schism and open confrontation but rather to the formation of two camps in the government that will advocate different solutions to pressing problems in line with their ideological preferences. This does not mean the country will undergo a general democratizing trend. The current political regime is likely to be conserved for to reproduce a new generation of elites by recruiting many Russians from the younger cohorts.

Our analysis sheds light on the impact of value changes on the behavior of future generations of Russian elites. Democracy does not generally seem to be the preferred form of government: authoritarian and/or technocratic governance are seen as equally acceptable political systems. Moreover, the popularity of authoritarian rule may even grow over time among both the elite and mass publics.

Finally, on the whole the younger generations are not very politically active. The 2011 protests are perhaps better understood as an emotional reaction or a fad, rather than a conscious decision to fully participate in the civil society. To be sure, there is a small segment of society – particularly in big cities like Moscow and St. Petersburg – that holds post-materialist views and is prepared to defend and promote its ideals. However, they cannot count on mass support, which they found out in late 2011-early 2012, when the protests fizzled out after an initial peak.

The rotation of elites over time may not necessarily lead to significant liberalization and democratization of the current political system. More likely, a combination of authoritarian and

technocratic methods will be employed. Civil society and democratic institutions will develop

albeit slowly, with economic concerns likely to be the main driver of the process – this process will be initiated by the need for better cooperation between the business people and the government. Increasing foreign investment and integration with international economic institutions will also likely play a role. However, for a significant segment of Russian society and the elite, democratization will not be of particular interest. Individuals born in the 1970s and 1980s who may be more post-materialist in their views will either be incorporated into existing government structures and adjust their political convictions accordingly or be sidelined from politics.

However, if economic growth resumes in the coming years, this will inevitably foster the spread of post-materialist values among younger Russians, especially those born after 1990. Greater numbers of post-materialists will translate into greater political activity. It will be difficult for the regime to ignore the growing calls for democratization and a more powerful civil society, forcing some concessions. Given Russia's growing integration with the international community, particularly on the economic front, and the institutional requirements that come with it, it appears that Russia's political climate may see some significant changes in the 2020s.

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Dynamics of binary choice on networks

SCIENTIFIC ORGANIZATION

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ABSTRACT

We consider the dynamics of binary decisions on graphs which takes into account local interactions and arbitrary stochastic component. We use the Master-equation to characterize the quantal response equilibrium in this model. In order to approach the equilibrium correlation behaviour, we use the annealed-approximation. On this way, we find typical timing of reaching the equilibrium, and discuss game-theoretic aspects of static and dynamic modeling approaches.

KEYWORDS

Graphs, networks.

ACKNOWLEDGEMENTS

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Inter-sector wage inequality and elasticity of substitution between skill-intensive products

SCIENTIFIC ORGANIZATION

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ABSTRACT

We study the response of the inter-sector wage inequality to shocks in demand. The analysis is based on a general equilibrium model with monopolistic competition in skill-intensive sectors and perfect competition in a traditional sector. Motivated by higher wages, workers aims to employ in skill-intensive sectors but face a risk to be unemployed because of labor market frictions: rejected job market candidates fail to find a job immediately.

KEYWORDS

Monopolistic competition; labor market frictions.

ACKNOWLEDGEMENTS

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SUMMARY

This paper examines the response of economies and, in particular, inter-sector wage inequality to shocks in demand. The analysis is performed by using a general equilibrium model with monopolistic competition in hi-tech sectors and perfect competition in a traditional sector. Hi-tech sectors are horizontally differentiated with respect to labor skills required by production technologies and to efficiency of these technologies. Motivated by larger wages, workers intend to work in hi-tech sectors but face a risk to be unemployed. Unemployment appears as a consequence of job market frictions: rejected skilled workers fail to find a new job immediately. The wages of employed workers are agreed through a bargaining mechanism.

As a result of monopolistic competition, the sector size is affected not only explicitly by consumers' distribution of spending but also implicitly by the elastic-

ity of demand in the sector. Redistribution of spending from traditional to hi-tech goods underlies the expansion of hi-tech sectors. This attracts new workers but because of sectors' limited capacity, a part of job market candidates is rejected, and the number of unemployment agents increases. *Variability of the elasticity of substitution (VES) between hi-tech goods implies* that a demand shift in favor of a *single* differentiated product affects the production of *all* sectors. This influence is based on changes in the *relative diveristy* of the differentiated products, which is the number of the product's representatives normalized by the sector size measured with consumers' spending. We posit that the economy can respond in two alternative ways: the relative diveristy of the differentiated products either enlarges or shrinks. In the first case, the demand for specific representatives of expanding varieties goes down. Having a limited monopoly power, firms higher price their goods compensating the shift in demand. Whole sectors incur a negative scale effect: the redistribution of the output to larger amount of firms with a fall of individual productions reduces the sector output. Sector, which produces the favored differentiated product, overcomes this effect and increases its output because of a direct influence of increasing spending for its goods. Following the output, the labor increases (decreases) in sector (respectively, in the other sectors) but the number of employees in each firm decreases. Hiring less workers, firms value each of them more and agree to increase their wages through the bargaining mechanism. Eventually, the inter-sector wage differential enlarges. In the second case, when the relative diveristy shrinks, we end up with the reverse prediction: the inter-sector wage differential decays.

The two responses of an economy are distinguished with consumers' elasticity of substitution between hi-tech goods. A decreasing leads to an increasing relative diveristy of the differentiated product, and vice versa. Intuition underlying this result is rather simple. We argue that spending additional money for specific goods, consumers exhibit a more elastic demand. The latter follows a growth/decline in demand for specific goods if σ is increasing/decreasing.

In our model, changes in the wage inequality are explored as a size effect, which is washed out under preferences with constant elasticity of substitution. On the other hand, the existence of an equilibrium is proved under preferences with relatively small VES. Nevertheless, the response of the wage inequality to a shift in tastes can be distinguishable. To our knowledge, this is the first attempt to estimate quantitatively the effect of VES in structural models with monopolistic competition. The scale of the response positively correlates with the efficiency of technologies in the corresponding industries, whose model proxy is the ratio of fixed to variable costs faced by firms.

ADDITIONAL INFORMATION

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Mosque as a place for adaptation and socialization of migrants

SCIENTIFIC ORGANIZATION

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ABSTRACT

The article explores the process of adaptation of Central Asia migrants in the Muslim community of Tomsk. Particular attention is paid to the role of Muslim clergy as a conductor into the local host society, as well as to the Russian language as a factor of interaction between migrants and locals. It is shown that it is in a mosque that migrants can get necessary information about employment and keep up-to-date with the latest developments in the world of Islam and Muslims. The article draws on interviews conducted in the congregations of the two Tomsk mosques and on expert interviews.

KEYWORDS

Migrant, mosque, community, adaptation, Russian language.

ACKNOWLEDGEMENTS

The project “Man in a Changing World. Identity and Social Adaptation: Past and Present” is funded by the Russian Government (grant #14.B25.31.0009).

SUMMARY

The religious perception of the world is one of the dominant factors that influence people’s minds today. The enhanced role of religion in Russia’s modern society has brought about the increased religiosity of the Russians. Due to sacredness, exclusivity and the concentration of ideas in a confined space, religious ties are much stronger than other forms of connection of people in a society. Despite the high level of development of modern society, science and technology, the religious factor still remains one of the main parameters of identity formation in people’s minds. In Islam, this identity is created in the form of ‘Ummah’ that is a world community of Muslims, part of which is constituted by the Islamic ‘Ummah’ of Russia and the Muslim community of Tomsk is, in turn, part of the Russian ‘Ummah’.

Studying the Muslim community of Tomsk can help identify the reasons underlying specific relationships among Muslims within it, as well as uncover the role of mosques as a place for communication and adaptation of Muslim migrants.

The Islamic religion is one of the major religions in the region of Tomsk. The history of the Tomsk Muslim community dates back more than 400 years. The Tatars of Tomsk that profess Islam have long inhabited the city. One of the main areas of their cultural presence here is called Zaistochie. In the Russian Empire, this was Tomsk Tatars’ traditional place of residence and it was here that their rites and customs had formed. There were places of worship (two mosques) along with cultural and educational institutions, a madrasah and a Turko-Tatar technical school present here as well.

After the collapse of the USSR in 1991, the Muslims of Tomsk embarked on a restoration of places of worship and their national autonomy. The two mosques were handed to them and they managed to have completely restored the buildings by the year 2015.

According to the 2010 Census, the number of local Tatars equated to 17029 which is 1,7% of the total population [1]. Only a small proportion of them go to the mosque. Year in year out, the number of Tatars, who know their national traditions and culture, decreases. Many families have long ago started to mix with the Russian population and have been assimilated. ‘We have a terrible assimilation going on in Tomsk. Here is a family, a big family. Half of them are Tatars and half are Russians. And now you cannot figure out who they are. Here are our children, our descendants, they are hybrids, that is what I call them. Some of them lean toward Christianity, others lean toward Islam. My nephew got baptized’. Some informants (for example, L.K.) do not see themselves as Tatars. There is also a factor of conversion to Christianity which is a departure from Muslim traditions. ‘She is Russian. Her father is Russian and her mother is Tatar, my sister. And so, they are two sisters, one of which did not get baptized. I went on a business trip to Kazan and brought some prayer-books to them. And to her I did not bring one. She had said she was a Christian. She took me to task. ‘Why did not you bring one to me? – But, Lyudochka, you said you were a Christian’. ‘But you do not know who I am in my soul”. And she does not allow baptize her daughter. Her daughter is 14 years of age. But the younger sister did get baptized as did her son. One family, one mother. But the father is Russian. Assimilation. What kind of ethnicity will their child be of? Unclear. On the one hand, they are Tatars, on the other – Russians’ [2].

Today’s ethnic composition of the Muslim community is essentially different from what it was a hundred years ago. If, in the early 20th century, there were local (Tomsk) Tatars and resettlers from the European part of Russia here, now, as censuses indicate, there are also migrants from the CIS countries, mostly from Central Asia, Transcaucasia and North Caucasus that is Azerbaijanis, Uzbeks, Tajiks, Chechens, Kyrgyz and Ingush people.

Number of migrants from Central Asia and the Caucasus in Tomsk oblast, based on censuses [3]

	1970	1979	1989	2002	2010	Proportion of the total population, %	
						2002	2010
Azerbaijanis	163	687	2752	4354	4178	0,42	0,40
Ingush	26	69	277	298	224	0,03	0,02
Kyrgyz	70	94	856	492	1427	0,05	0,14
Tajiks	35	165	912	498	956	0,05	0,09
Uzbeks	247	1065	3328	1626	3924	0,15	0,37
Chechens	65	166	487	711	547	0,07	0,05

According to the Tomsk Statistics Service's data for 2015, there is a further increase in the number of migrants from the CIS and other countries of the world: from Azerbaijan – 324 people, from Kyrgyzstan – 511, from Tajikistan – 310, and from Uzbekistan – 929 [4].

Migration to the region of Tomsk has largely changed the profile of the local Muslim community. The understanding of Islam has changed accordingly, as rites and religious practices exercised by Central Asia Muslims are much stricter than the ones exercised by Tatars including, for example, some of the elements of the Mohammedan prayer.

Religious boards that are based at the city's mosques are headed by Muslim migrants as well. Imam of the Red mosque is Tajik, and Imam of the White mosque is Kyrgyz. The Tomsk Imams form their religious space differently. Preaching by the one differs from preaching by the other. The Imam of the White mosque preaches in Kyrgyz and in Russian. The Imam of the Red mosque preaches in Russian. The ways preaching is carried out are also different.

Today, the Muslim community of Tomsk is ethnically heterogeneous; it includes people from various ethnic backgrounds who profess Islam. To communicate, they use their national languages – Tatar, Kazakh, Uzbek, Tajik, and Caucasian languages. In order to learn about Islam, consult the Muslim clergy, understand preaching at the mosques as well as to interact with the authorities, they use the Russian language. Knowledge of Russian helps the community not only adapt to local specificities of the religious space but also to get better integrated in the host society.

Our further research aims to test, drawing on the case of Tomsk, the hypothesis about the formation of a 'Russian Islamic sociolect' and its role in the adaptation of Muslim migrants. This sociolect includes several variations (Arabization, Russification), each of which has its own forms of using Islamic terminology, borrowing directly from Arabic, doing literary translation into the Russian language, etc. It is noteworthy that certain variations are not specific to only one group (be it social or political group) within the Islamic discourse and can be used by different actors, even by potential rivals (e.g. rival muftiates or two competing mosques) [5].

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Sokolov Sergey
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Senior Researcher

The idea of the Novgorod Republic and European influence on 18th century Russian historians

SCIENTIFIC ORGANIZATION

Ural Federal University

ABSTRACT

The paper concerns the issue of the emergence of republican ideas in 18th century Russian historical writings as well as the aspects of European influence on Russian thinkers.

KEYWORDS

European Innovations, the Novgorod Republic, Historiography, Intellectual History.

SUMMARY

The lecture will introduce some outcomes of the research project investigating the very first steps of the classical republican discourse on Russian soil. During the 18th century Russian intellectuals were gradually becoming familiar with different patterns of republicanism. They learned key points of republican theory, such as liberty, virtues, the necessity to stand up for rights and for the republic, and against the danger of corruption. Having completed a thorough reading of Greco-Roman texts, Russian historians, political thinkers and litterateurs in the second half of the 18th century were able to apply classical plots and patterns to the Russian past and present. They considered different episodes of Russian history as a struggle between republicans and monarchists and started to recognized Novgorod and Pskov as two powerful ancient republics. Until the 1790s, none of the intellectuals sympathized openly with republican ideology, they all argued for the monarchy. Nevertheless, they were attracted by the republican discourse.

Along with the philosophy of the Enlightenment and the French Revolution, such republican discourse served as a springboard for Alexander Radishchev and some of the Decembrists as they put forward a genuine republican ideology in the last decade of the 18th and the opening years of the 19th century. These new thinkers considered the monarchy weak and imagined Novgorod as a good example of a powerful and virtuous republic, whose existence gave added impetus to the possibility of republican government in the not too distant future.

Sorokin Alexander
Candidate of historacal sciences
Senior Research Fellow

"Homo universitatis": dynamics of the corporate identity of Russian university lectures in the 1990-2000-ies

SCIENTIFIC ORGANIZATION

Tomsk State University

ABSTRACT

Under circumstances of globalization and transformation of Russian society the identity crisis is taking its toll. In this respect, the research of university research and teaching community as a special category within Russian society becomes pertinent. On the basis of published sources our previous ethnographic research conducted in 2014-2015 among university lecturers of Tomsk universities factors that influenced the formation of corporate identity of Russian university lecturer's community in 1990-2012 have been analyzed.

KEYWORDS

"Homo universitatis", corporate identity, identity crisis, higher education, post-Soviet Russia.

ACKNOWLEDGEMENTS

Written in the framework of the project the project "Man in a Changing World. Problems of identity and social adaptation in history and at present" (the RF Gov-

ernment grant No. 14.B25.31.0009); “Homo Universitatis”: the phenomenon of Siberian academic community in the late XIX - early XXI centuries (Grant of the President of the Russian Federation for state support of young scientists and leading scientific schools of the Russian Federation No. MK-5402.2016.6); the project “Social forms of science organization in Siberia in the 1941-1991-ies: the meaning and role in social, cultural and economic modernization of the Soviet society” (FFH grant No. 15-33-01331).

INTRODUCTION

Under circumstances of globalization and transformation of Russian society the identity crisis is taking its toll. This crisis is caused by the collapse of foundations and values of Soviet period and the loss of historical ties with traditions of Russian nationhood. No less significant is the realization of importance of acquirement and maintaining of new identity in globalizing world. In this respect, the research of university research and teaching community as a special category within Russian society becomes pertinent. Despite its relative small number, by the beginning of the XIX century, this social group started to play a significant role in Russian public life and of served as a marker of political and social processes.

Historical reconstruction of evolution of academic teaching community and profession of university lecturer taking into account social transformations in the country, allows us to fully comprehend consistent patterns of these transformations, trace trends that influence current situation and forecast contours of the future changes in the profession.

MATERIALS AND METHODS

The study of corporate identity of Russian university lecturers lies on the borders between history, anthropology, sociology, psychology and pedagogy. We will use the theory of social construction by P.Berger, T. Luckmann because it encompasses multidimensionality and dialectical character of the process of constructing identity where the subject of its construction is simultaneously the object.

The main sources that were used for this research are published (laws and normative-legal acts of the Ministry of science and education of RF) and unpublished material (archival documents, including documents of management and record keeping), periodicals, ego-documents (diaries, letters and memoirs). One of the key sources were the results of interviews with representatives of the academic community of Tomsk, conducted in 2014 and 2015.

RESULTS

Global social and political transformations in 1990s have had a considerable impact on the Russian teaching community, that has undergone a new crisis of corporate identity. From the point of view of corporate identity of university teaching community, it seems important to put emphasis on the analysis of factors that influenced the formation of corporate identity of university lecturers in Russia in 1990-2010s.

As a result of this research we have discerned negative, positive and neutral (dual) factors.

Negative factors (hampering the formation of corporation). It is important to mention circumstances that negatively influenced the formation of corporate identity of university lecturers. In our view, among those circumstances are the following:

- demographic situation in the country;
- holding of more than one office;
- reduction of a repertoire of traditional corporate events

Neutral (dual) factors. Among these circumstances are the following:

- the emergence of lecturers of a new kind
- feminization of teaching staff
- university autonomy

Among **positive factors**, that are beneficial for the formation and enhancing university corporate identity are:

- the practice of formation of corporate culture of universities;
- the rise of prestige of profession of university lecturer;
- -self-recruiting

CONCLUSION

Nowadays the corporation of university lecturers faces new challenges that could possibly turn to both dangerous perils and new opportunities. Two scenarios seem are most likely. First assumes that differentiation of universities would lead to gap between lecturers working in leading universities (Leading research university (VIU), National research universities (NIU), federal universities) and outsiders. In case they can not manage to adapt to new reality, lecturers from second group universities will have to leave their jobs, which in turn will jeopardize the system of education. The second scenario considers that reforms will lead to qualitative renewal of corporation and rise of level of its identity, and lectures of universities of the first group will become locomotives of this process.

ADDITIONAL INFORMATION

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The role of information in conflict escalation

SCIENTIFIC ORGANIZATION

New Economic School, NRU Higher School of Economics

ABSTRACT

We consider a continuous incomplete information escalation game. We assume that two competitors are engaged in a brinkmanship game such that at any moment each of them can either continue escalation or back down: if the escalation level reaches some threshold (unknown to the players), disaster (war) breaks out. We derive two comparative statics results. First, as contesters become less certain about the value of the benefit from winning the conflict, the probability of peace increases. Second, as players' signals grow more positive-dependent, the probability of war increases.

ACKNOWLEDGEMENTS

Joint work with Eyal Winter, Hebrew University of Jerusalem.

Taran Ekaterina

Researcher

Subjective wellbeing in older adults living in Tomsk Region

SCIENTIFIC ORGANIZATION

National Research Tomsk Polytechnic University

ABSTRACT

This study investigates the subjective wellbeing of older adults living in Tomsk Region. We administered 2 questionnaires. In each questionnaire 600 respondents (aged 65 years or over) were interviewed face-to-face. We evaluated how life satisfaction is affected by demographic factors (eg., age, gender, etc.), social aspects (e.g., social network, isolation and comparison, etc.), psychological characteristics (e.g., depression, dispositional optimism). Both questionnaires provided new and interesting insights about the subjective wellbeing of Siberian older adults.

KEYWORDS

Survey; Cross-sectional study; Subjective wellbeing; Life satisfaction; Older adults; Tomsk Region.

ACKNOWLEDGEMENTS

This work was performed by the author in collaboration with Tomsk Polytechnic University within the project in Evaluation and enhancement of social, economic and emotional wellbeing of older adults under the Agreement No.14.Z50.31.0029.

INTRODUCTION

Twenty-eight percent of the Russian population will be aged 60 years or over by 2050. This demographic phenomenon change will generate socio-economics and political challenges that will require to better understand the factors affecting subjective wellbeing in older adults. In this study we aim at exploring which variables affect the subjective wellbeing (e.g., life satisfaction or happiness) of older adults living in Siberia. More precisely we interviewed older adults living in Tomsk Region. This region has a population of about 1 million people, and twelve per cent of them (approximately 50.000 people) are older adults. Little research has been conducted on subjective wellbeing of Siberian older adults. Therefore, this study provides original and new data concerning the quality of life of these older adults.

Subjective wellbeing reflect the psychological aspect of the global experience of one's life. For older adults, a high level of subjective wellbeing has been associated with successful ageing, and thus with many positive outcomes, like for example good health and being economically self-sufficient. In this study we investigated two important components of subjective wellbeing: life satisfaction and happiness. Life satisfaction refers to the cognitive-judgmental aspects of subjective wellbeing; whereas happiness refers to the affective and emotional aspects of this construct. These two components measure closely related but distinct aspects of subjective wellbeing and thus can provide an evaluation of which factors affect overall quality of life from two different points of view, a cognitive evaluation of respondents' situation and a description of their feelings.

Life satisfaction and happiness are associated with a large number of socio-demographic factors. In this survey, we included questions related on the factors that, according to the literature, showed to have a strong impact on subjective wellbeing. Therefore, the following factors have been included in our survey: social support (e.g., provide or receive help from people they are close to), social activities (e.g., taking care of grandchildren), emotional support (i.e., feeling appreciated by close people), self-reported health, economical situation, age, gender, marital status, education level, and the place of living. In the analyses these factors have been used as possible predictors of life satisfaction and happiness.

In this study we administered a questionnaire to older adults living in Tomsk Region. The aim was to identify the factors affecting their subjective wellbeing (i.e., life satisfaction and happiness). Life satisfaction and happiness have been considered as independent constructs and analyzed in two separated logistic regressions. A second questionnaire will be administered in June/July 2016. This second questionnaire aims to further investigate some aspect that showed to be significantly related with subjective wellbeing in the first questionnaire.

METHODS AND MATERIAL

Respondents and Procedure

A cross-sectional study was conducted in Tomsk Region (Siberian Federal District, Russia). We administered a questionnaire through face-to-face interviews conducted in respondents' homes. Six hundred respondents were randomly recruited through quota sampling. All respondents were aged 65 years or over. In each family unit, only one older adult was interviewed. All interviews were conducted in Russian by mother-tongue interviewers. Each interview lasted 40-60 minutes. Verbal informed consent was obtained from all respondents prior to the interview. Each respondent received a standard set of gift (e.g., tea, chocolate, etc.) for the participation.

The questionnaire was carried out between August and September 2015 by an organization with experience in survey research. The questionnaire included 99 items aimed at investigating difference aspect of older adults' life. To investigate which factors are associated with life satisfaction and happiness in our sample, we selected a sub-set of these questions. More precisely, we selected the questions relating to social aspects and demographic characteristics.

Of the 600 questionnaires, 111 had missing responses on one or more variable of interest, and thus were excluded from the analysis. Therefore, the final sample included 489 respondents.

A second questionnaire will be carried out in June/July 2016. The methodology and the procedure will be the same as for the first questionnaire. A new sample of 850 respondents living in Tomsk will be interviewed.

Measurements

Some of the questions were originally in English. These questions have been translated into Russian using the standard method of back-translation. Two separated logistic regression have been performed, with the following two dependent variables: Life satisfaction and happiness.

The predictors (i.e., independent variable) were questions that investigated the following factors: Caring for your children and grandchildren, receiving and providing social support, emotional support, self-rated health, satisfaction with standard of living, age, gender, marital status, educational level, and residence area.

Similar analyses will be performed on the second questionnaire.

RESULTS

The mean age of respondents was 74.4 year (SD=6.9), with 324 women and 165 men. The mean value of life satisfaction was 5.9 (SD=2.4) and the mean value of happiness was 6.2 (SD=2.1). The correlation between life satisfaction and happiness was 0.55.

Life satisfaction was significantly associated with the following factors: Self-reported health; satisfaction with standard of living; place of living; receiving help; taking care of children and grandchildren; emotional support.

Happiness was significantly associated with the following factors: Self-reported health; providing help; emotional support.

DISCUSSION

In this study we investigated which factors are related with life satisfaction and happiness, which are two important components of subjective wellbeing. Consistently with the literature, we found that different socio-demographic variables are associated with life satisfaction and happiness. Our results contribute to show that life satisfaction and happiness are similar but different components of subjective wellbeing. In fact, the predictors of these two components only partially overlap, and thus it is useful to measure both these components to have a global view of subjective wellbeing.

The follow-up questionnaire, that we will administered in June/July 2016, will provide further evidence on the factors affecting subjective wellbeing. In this second questionnaires life satisfaction and other factors will be measured by means of Likert scales. This will provide a more precise measure of subjective wellbeing. Moreover, we will translate and adapt to Russian language some Likert scale, which have been developed in English but not yet tested and validated in Russian language. These scale will furnish Russian researchers with new measures useful to study subjective wellbeing and to compare the results with those of other countries.

Terekhina Olga
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Psychological characteristics of women undergoing in-vitro fertilization treatment

SCIENTIFIC ORGANIZATION

The Laboratory for Cognitive Investigations and Behavioural Genetics, International Centre for Research in Human Development, Tomsk State University

ABSTRACT

Research into psychological characteristics of women preparing for motherhood after IVF treatment has important practical implications. There are large individual differences in psychological states among women during this period. The results showed that mental state of the majority of women undergoing IVF treatment was characterized by an acceptable level of anxiety, aggression and rigidity, and good resistance to failures and difficulties. The dominant reproductive motives included: “For social status”, “For the feelings of motherhood”, and “To fulfill the need for love”.

KEYWORDS

Women, infertility, IVF treatment, psychological characteristics, reproductive motives.

SUMMARY

Research into psychological characteristics of women preparing for motherhood after IVF treatment has important practical implications. Psychological characteristics can mediate the level of stress associated with the experience of infertility, cause psychogenic forms of infertility, and moderate psychological consequences of infertility. In turn, these consequences may affect treatment outcomes, act as etiological factors in the development of borderline mental disorders, determine the success of childbirth and influence subsequent development of the child. Despite stressful conditions leading to IVF treatment and the stress of the treatment itself, there are large individual differences in psychological states among women during this period. The sources of these differences remain poorly understood.

The study involved 214 women diagnosed with infertility, undergoing IVF treatment. Women filled out questionnaires using the following diagnostic tools: The Eysenck Personality Questionnaire (EPQ), the Spielberg-Hanin scale of anxiety, the *Beck Depression* Inventory, and a questionnaire about reproductive motives “My pregnancy”.

The results showed that mental state of the majority of women undergoing IVF treatment was characterized by an acceptable level of anxiety, aggression and rigidity, and good resistance to failures and difficulties. Only 30% of women showed symptoms of minimal, mild, moderate, and in rare cases – severe depression. However, the majority of women in showed high level of trait anxiety. The dominant reproductive motives for this group included: “For social status”, “For the feelings of motherhood”, and “To fulfill the need for love”.

Significant correlations between the length of planning time and level of frustration among women were identified. However, the women did not differ in their psychological characteristics as a function of the number of treatment attempts and success of the treatment.

The results are discussed in the context of existing literature and the latent factor structure of mental states, trait anxiety and reproductive motives that emerged from the data.

ADDITIONAL INFORMATION

Olga Terekhina, Tatiana Bokhan, Anna Ulianich, Marina Shabalovskaya, Maria G. Tosto, Yulia Kovas.

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Leading research fellow

Do we go shopping downtown or in the 'burbs?

SCIENTIFIC ORGANIZATION

Higher School of Economics (HSE)

ABSTRACT

We combine spatial and monopolistic competition to study market interactions between downtown retailers and an outlying shopping mall. The market solution stems from the interplay between the market expansion and the competition effect. Firms' profits increase (decrease) with the entry of local competitors when the former (latter) dominates. Downtown retailers vanish swiftly when the mall is large. A predatory but efficient mall need not be regulated, whereas the regulator must restrict the size of a mall accommodating downtown retailers.

KEYWORDS

Shopping behavior; retailers; shopping mall; spatial competition; monopolistic competition.

ACKNOWLEDGEMENTS

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Comparing socio-demographic, psychological and health characteristics across families using natural conception vs. IVF conception: evidence from the Russian genetically informative pregnancy cohort

SCIENTIFIC ORGANIZATION

Psychological Institute of Russian Academy of Education

ABSTRACT

The purpose of the Russian genetically informative pregnancy cohort is to support research into genetic and pre- and postnatal environmental effects on child health and mental development. In this talk we present the preliminary analysis of the first 200 families with naturally conceived and IVF pregnancies. By employing an IVF design it is possible to disentangle not only the relative effects of genetic and environmental factors on development, but to parse the environment into prenatal and postnatal components.

KEYWORDS

Longitudinal study, IVF, child development, genetics, pregnancy.

ACKNOWLEDGEMENTS

This study was funded by the Russian Science Foundation (grant RSF № 14-48-00043).

SUMMARY

Early childhood experience has long-term effects on individual trajectories and outcomes, including a child's learning ability, academic achievement and the overall quality of life (e.g., Boivin, & Bierman, 2013). Therefore, it is crucial to understand the mechanisms of early child development to improve the lives of the future generation.

The purpose of the Russian genetically informative pregnancy cohort is to support research into genetic and pre- and postnatal environmental effects on child health

and mental development. Data on biological (DNA, trace elements), socio-emotional and physical characteristics of parents and children are collected prospectively starting from pregnancy. The project combines the traditional longitudinal method with a novel design based on families in which children were conceived through in vitro fertilization (IVF). Children conceived by homologous IVF, egg donation, sperm donation, embryo donation and surrogacy differ in the extent to which they share genes with their parents. By employing an IVF design it is possible to disentangle not only the relative effects of genetic and environmental factors on development, but to parse the environment into prenatal and postnatal components.

In this talk we present the preliminary analysis of the first 200 families with naturally conceived and IVF pregnancies at Time 1 (12-13 week of pregnancy) and Time 2 (33-34 week of pregnancy). We investigated potential differences between IVF and non-IVF parents on a number of characteristics, including demographics and risk factors such as state of health, smoking and alcohol consumption, and psychological characteristics. These will be taken into account in the future analysis of prenatal predictors of child development.

Abstract submitted from the Laboratory for Cognitive Investigations and Behavioural Genetics, International Centre for Research in Human Development, Tomsk State University.

ADDITIONAL INFORMATION

Chairs: Yulia Kovas and Elena Grigorenko

Irina Voronina, Elaine White, Anastasia Karetina, Inna Feklicheva, Sergey Malykh, Gordon T. Harold, Michel Boivin, & Yulia Kovas.

Weber Shlomo
PhD
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SCIENTIFIC ORGANIZATION

New Economic School

Measurement of socio-economic diversity

KEYWORDS

Diversity

ACKNOWLEDGEMENTS

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SCIENTIFIC ORGANIZATION

National Research Tomsk State University

«3D Revolution» in Archaeology in Russian Perspective

ABSTRACT

The last decade has introduced methods of three-dimensional documentation and rendering of information uncovered by excavations, opening up entirely new opportunities in presenting scientific discoveries and bringing home their significance to the public. Unfortunately, however, laser scanning and close-range photogrammetry have not yet gained due currency in Russian archaeology. The report will present the latest results of the application of 3D documentation and 3D visualization techniques in archaeological and museum projects of Tomsk State University.

KEYWORDS

Archaeology, 3D scanning, terrestrial photogrammetry, 3D visualization.

ACKNOWLEDGEMENTS

This research was performed as part of the project “Man in a Changing World. Problems of Identity and Social Adaptation in History and at Present” (Russian Government Grant № 14.B25.31.0009).

SUMMARY

The last decade has introduced methods of three-dimensional documentation and rendering of information uncovered by excavations, opening up entirely new opportunities in presenting scientific discoveries and bringing home their significance to the public. Now, photorealistic interactive 3D models make it possible for anyone to see archaeological sites. Stereoscopic videos displayed by specialized museum equipment create a total participation effect, enabling any visitor to watch excavations step by step, in all their detail and from all perspectives. Unfortunately, however, laser scanning and close-range photogrammetry have not yet gained due currency in Russian archaeology. The report will present the latest results of the application of 3D documentation and 3D visualization techniques in archaeological and museum projects of Tomsk State University.

1) Timiryazevo burial site: A 3D recording project.

A 3D-recording project was brought into practice by Tomsk State University during the investigation of Timiryazevo burial site (5th–10th centuries AD) in 2014. During the excavation, three-dimensional records of the whole archaeological site were made at each stage, as well as individual records of all artifacts. 3D recording was provided by the SFM technology. The data obtained was used for research and was also applied in the development of the exhibition project «Secrets of Timiryazevo Burial Site: The Circle of Life and Death in Siberian Shamanism». The exposition revolves around unveiling the meaning of the rite of burying lookalike dolls of the deceased, which was practiced by many indigenous peoples of Siberia. The exposition is designed to let the visitor go through the whole cycle of knowledge extraction together with archaeologists, “detectives of the past”: from a bunch of strange miniscule objects found in the sand to reconstruction of the whole sophisticated rite of “ultimate funeral” including the burial of the deceased’s lookalike doll. The tools used to develop the topic included a stereoscopic video created with Autodesk 3D Studio MAX 2014 and displayed in the exhibition.

2) 3D Recording of a 19-Century Ob River Ship.

A 3D recording of a 19-century wooden ship discovered on the bank of the river Ob (Western Siberia) was performed in autumn 2015. The archaeologized ship was partly under water, partly lying ashore, buried under fluvial deposits. The 3D recording was performed in October, when the water level was at its lowest after clearing the area around the ship. A 3D recording at the place of discovery was required as part of the ship museumification and reconstruction project. The works performed were primarily aimed at preserving as much information about the object as possible.

Given the location and peculiar features of the object, a combination of close-range photogrammetry and aerial photography was considered to be the best possible solution for creating a high-quality 3D model.

The dismantled ship was delivered to Nizhnevartovsk Museum of Local History in October 2015. The ship is going to be reassembled using the created 3D model to be exhibited in the museum. The resulting models are also going to be used to make a virtual 3D reconstruction of the ship in the future. We shot a stereoscopic video for Nizhnevartovsk Museum of Local History to let visitors see the place of discovery and explore the ship in greater details. Besides, 3D printing allowed for creating a miniature of the ship, which is also going to be included in the exposition devoted to this unique discovery.

3) 3D Reconstruction of Koch, Russian Rowing/Sailing Boat of the 17th Century.

Koch is a Russian rowing/sailing boat adapted for the heavy Arctic conditions. A virtual 3D reconstruction of a 17th-century koch commenced in 2014.

Precise engineering drawings were unknown to Russian boat makers of the 17th century, while the few pictures of koch and inconsistent written sources do not allow for an authentic reconstruction of all details and specific features of the vessel. The original boat parts discovered during archaeological studies in Mangazeya, the first transpolar Russian town in Siberia, served the unique resource for the reconstruction.

The area had no forests to provide wood for construction, so houses were built from dismantled boats. Structures built entirely from framings were surveyed in Mangazeya. Boat parts are perfectly preserved in the cultural layer of permafrost. For the purposes of reconstruction, we used the two best preserved koch framings dating back to the 17th century.

We needed to perform 3D scanning of 293 boat parts. Those parts represented individual pieces of various forms and sizes (from 0.3 m to 5.6 m). This diversity was the key factor when choosing the equipment and elaborating scanning methods. We used scanners GoScan 3D and GoScan 50 by Creaform with the optimal resolution of 1 mm. Textures were identified using photo camera Nikon D700 and the SfM (structure from motion) 3D model technique. Agisoft Photoscan Pro software was used to create low-poly models with applied textures. We used Geomagic Wrap software to perform the final processing of the scanned model and to copy the textures from low to high poly. 3D Studio max software was used to reproduce the original look of the parts by removing traces of secondary use and natural wood deformation. The same software was used for virtual assembly of the parts and 3D reconstruction of the whole boat.

The shift to a digital culture in archaeology represented by this and other recently developed recording systems represents a new paradigm in archaeological practice and offers many opportunities. Compared to the traditional manual registration methods, the improvements of the new methodology have not only an economic, time efficient and cost-effective importance but also a major scientific value. With an abandonment of both the tools and spatial divisions of traditional archaeological excavation, we may be describing the most radical change to archaeological practice since the introduction of structured excavation and recording over a century ago. From the late parts of the 19th century up to today, the development of spatial documentation has been phenomenal. But it is only in the last 10-20 years that we have been able to fully utilize the potential of digital recording methodology as a cost-efficient means of spatial documentation in archaeology. The most recent developments in field documentation methodology, such as digital photogrammetry and laser scanners, especially have shown great potential for archaeology in general. New ways of using and interpreting the data gathered have started to make their impression on archaeology, although this is merely the beginning of a «digital revolution» in archaeology. This clearly illustrates the importance and long-term benefits of using modern 3D recording techniques in field archaeology. However, Russian archaeologists are as yet mostly unaware of their availability, so they currently hardly ever use them.

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European project on Russian soil: History of Russian Red Cross

SCIENTIFIC ORGANIZATION

Ural Federal University

ABSTRACT

The paper analyses the history of Russian Red Cross from its origin up to 1918. It shows how initiative of Henry Dunnant receipted by Russian imperial elite had been implemented and how activity of Red Cross had influenced on social and political development in Russia.

KEYWORDS

History of Russia, European influence, Russian Red Cross.

SUMMARY

Based on the vast materials presentation focuses on the history of founding Russian Red Cross (RCC) and reconstructing its evolution at the second half of the XIXth century. It also aimed on identifying major ideas and practices adopted from the Western experience. Another purpose of the study is to define how did Russian Red Cross changed charity practices and the mode of interactions between army, state and society. In conclusion the research outlines major mechanism of penetrating and adopting new practices from imperial center to the provincial level.

Ideas of Henry Dunant of establishing International organization aimed on providing assistance for wounded can be labeled as unique ones. Russia had both had experience of nursing (at the Crimean War) and involvement of civil society in charity issues. Dunants' initiative was innovative because it contributed to lessening States monopolistic control over all aspects of waging and conducting the war. Thus founding the Russian Red Cross can be regarded as the attempt to broaden civil society involvement at the war issues. The process is very much obvious at the era of mass-conscripted armies and industrial warfare.

Experience of European countries, especially Prussia and France was extremely important on development of the structure and practice of Russian Red Cross. Although it was founded by representatives of upper class, soon regional elites and fractions of Russian bureaucracy and intelligentsia started to take part.

What did the Russian Red Cross change? How did its activity influence the social and political life of Russian Empire? Definitely the RRC's activity had multiple effects and manifestations. The most important are summarized below:

The RRC contributed to introduction of new approaches to health care of wounded as well as more systematic, organized approach, adoption of technical and scientific innovations in military medicine.

Involvement in the RCC activities provided new opportunities for the education of women and expanding the scope of women's participation in public life and the scope of their employment.

The Russian Red Cross as an organization gave to its members the feeling of participation in large political processes. Working and supporting the RRC activity can be regarded as s special way to demonstrate patriotism, applicable to all social strata and classes.

Inevitably activity of Russian Red Cross had become one of the themes for the official propaganda, the new means of constructing the image of Russia as progressive and westernized state.

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The Rise and Fall of the "Russian Techie" Brand in London

SCIENTIFIC ORGANIZATION

European University at St. Petersburg

ABSTRACT

Russian IT professionals developed and used the "Russian techie" brand – which I use as a distinguishing mark of professional competence and status – to facilitate their careers outside of Russia. Highly skilled migrants with a particular training, they thought of themselves as part of a specific and recognizable community, which gave them an incentive to continue to promote and disseminate the recognition of the brand associated with that community.

KEYWORDS

Russian Techies, Language Community, Professional Migration.

ACKNOWLEDGEMENTS

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SUMMARY

Russian IT professionals developed and used the "Russian techie" brand – which I use as a distinguishing mark of professional competence and status – to facilitate their careers outside of Russia. Highly skilled migrants with a particular training, they thought of themselves as part of a specific and recognizable community, which gave them an incentive to continue to promote and disseminate the recognition of the brand associated with that community. I use biographical materials to

uncover professional paths, career patterns, and changes in the self-identification of Russian IT professionals who decided to migrate to London tracing the transformation of their self-representation through the narratives they themselves give about their training, experience and migration strategies, as well as their integration into local culture and professional communities.

As a brand, the "Russian techie" trademark was first recognised only among Russian professionals themselves – people who had performed successfully as computer scientists and programmers. At first an image of self-identification and pride, reputation for competence soon moved beyond those confines to become a widely recognised stereotype. Of course, this brand could play a positive role in the careers the "Russian techies" only if the actual IT specialists lived up to the expectations set by it. A further challenge to the staying power of the brand was posed by the growth and differentiation of the community itself, requiring more efforts to keep high quality standards across the membership of its various growing sub-communities. To understand the rise and fall of the "Russian techie" brand we need to trace the crucial turning points in the migration patterns, first from the USSR, and then from Russia, to London: the collapse of the Soviet Union in 1991, the "dotcom bust" and the institution of the HSMP visa regime in 2001-2002, and the discontinuance of the HSMP programme in 2011.

The educational background of Russian computer specialists was crucial to their self-identification and group solidarity, and thus is key to understanding how the "Brand" emerged: *"We [Russians] have very talented people" (M, 40, professor).* This pride emerged from a shared cultural background and a specific pattern of training and education. The Soviet heritage of computer science (or informatics) shaped the future development of academic and industrial fields in Russia, and especially its educational component. I do not mean just the teaching of specific skills, but a general pedagogical approach where charismatic leaders played a crucial role. However, it was not only the teacher who "shapes the student's brain", but the whole curriculum that aimed at instilling a special "way of thinking", "attitude of mind", "mindset" – notions which are often used by my informants to describe the difference between themselves and specialists from other countries, and to show how they feel about having grown up in Soviet schools.

By virtue of the excellence of their training, Russian CS and IT professionals perceive themselves as elite professionals with their own working ethics and discipline. This pride is rooted in the Soviet educational system, where mathematical disciplines serve as the core of the curriculum, and where those who were interested in or curious about technical tinkering were afforded numerous opportunities to do so. Though this training did not guarantee that each professional had the same ability or the same technical aptitude, empirical data does provide grounds for the hypothesis that the Soviet education encouraged specific skills and the ways of thinking: *"Russians went through a unique school training"* (M, 38, COO). Schools and Departments of Mathematics and Physics imbued social activities with educational content: *kruzhki* (circles or study groups as a part of extracurricular activity) for kids, Olympiads and contests for secondary schools and universities, outdoor activities and camps for Math classes – these were all aspects of the Soviet training systems in Mathematics, Physics, and Computer Science. The social networks created by these activities and the attachment to the institutions that nurtured them facilitated individual success for many of their participants.

The superior skills of many who underwent this education became clear when Russians began to compete abroad with IT specialists from other countries, especially those from India. In the era of mass outsourcing, Steve Chase, former President of Intel Russia once said: "The policy we have at Intel is simple. If we can, we commit difficult problems to engineers in the USA. If the task is very labour-intensive, we assign it to the Indian specialists. If the problem cannot be solved, we offer it to the Russians". This kind of respect for the "brand" enhanced its visibility on the map of the global labour market.

As the borders between East and West opened, London became a prime destination for Russian computer specialists. There were many factors which made it attractive to Russians. First, it, already seemed familiar through the experience of colleagues, and the legends that the "imaginary West" (Yurchak 2005) promised a comfortable life and a successful career. London also seemed not just a place of opportunity, but a place of stability. It is a global city (Sassen 1991), where a strong financial system offered top-paying jobs and challenging tasks.

In this competitive market (Ewers 2007), Russians quickly began to distinguish themselves. They became visible in ways that other ethnic groups were not: the

phenomena of 'Russian lunches' and 'Russian mafias' (in the benign sense of Russian professional groupings) appeared in the areas of high concentration of banks – in the City of London or the Canary Wharf section. This visibility, enhanced by extraordinarily high competence and superior performance of the early arrivals, incubated the "Russian Techie" brand, and attracted still more émigrés to London.

So who were the typical bearers of the "Russian Techie" brand? They were (and still are) generally young – from 25 to 35 years old. Their communities were male-dominated, and were generally composed of former or current co-workers and friends with the same profession and leisure interests, mainly outdoor activities like hiking or travelling. They were politically active, interested in the political situation in Russia, and often held largely oppositional views. Many were still emotionally attached to home-country, keeping up with events there, and maintaining contact with home through friends and relatives. Some of them had experience of long-term work in other countries, and some were "serial migrants," changing their country of residence every 3-5 years (Ossman 2013). They constituted a mobile cadre of 'Russian techies', for they were often contract workers, self-employed and responsible for their own taxes, social security, and other aspects of work. In general their position was relatively precarious: *"A contractor usually earns more, but there is no promotion track. It is consumable material" (M, 44, System administrator).* Yet an active system of recruitment agencies and headhunters usually guaranteed that a new job would be awaiting when an old one ended.

While the majority of HSMP/Tier 1 holders maintain some association with the Russian community or other IT professionals, many of them remain invisible. Single individuals often prefer not to be a part of community, but rather to dissolve into the IT market and cultivate their own professional careers. And while they often keep in touch with friends from their home country and with co-workers, these independent IT specialists might be viewed as authentic global professionals in the local IT market, because they are not particularly interested in maintaining Russian connections.

The institutionalization of practices during the process of emigration had a great influence on life in London for the third wave IT émigrés. Being part of a Russian community from the very beginning, they remained within that community and participated in its various events and meetings. And since the flow was large in comparison with previous waves, the number of communities and participants grew rapidly and differentiated, transforming status of IT specialists from creative techies into office workers owing to job rotation, short contracts, or self-employment: *Still it seems to me that banks… they pay a lot of course, but in many respects… you know, what I call them? … Golden cage. Not just for traders, but finally for us [IT-guys] as well, yes. I mean, you are being bought, put in the cage (M, 36, Programmer).*

So the "golden era" of IT migration quickly turned into the "golden cage" of corporate employment: real freedom to change workplaces tends to be imaginary. One needs to face the problem of changing projects and of arranging social services and social security with every new job. For banks and companies, these professionals represent a pool of relatively cheap labour (in comparison with permanent workers). For the employees, the banks represent willing employers – good jobs always seemed available. Yet these IT specialists become ordinary (though highly paid) corporate workers, one of thousands others like them. In In this bargain, they gain steady employment opportunities, but they give up any sense of stability in their careers. The same story repeats itself with communities where IT professionals interact.

You used to be, you know, exclusive. But now there are plenty of that sort. The element of exclusiveness had been lost… You used to come to some new hangout, on a visit, and you discovered 80% of your people, meaning, your were familiar with… The circle was fixed… Now, when you come somewhere, 90% of people, you don't know them. All of them are new to you… The structure of all Russians, of the Russian community, if I may voice such global conclusions, it is a quite clear and known trend, because of so many people coming (M, 37, Developer).

As IT specialists grow in number, they create new networks, which attract not only "exclusive" professionals, but also "craftspeople," meaning people of average level of skills. It is a case when quantity trumps quality in general, and this dynamic leads to negative effects. To be a temporary worker in the labour market means sacrificing any aspiration to improve one's status: *"they don't want to learn new things; they find no zest left in life" (M, 35, Developer).* If the high level of performance fails to be sustained, the "brand" decreases in its value.

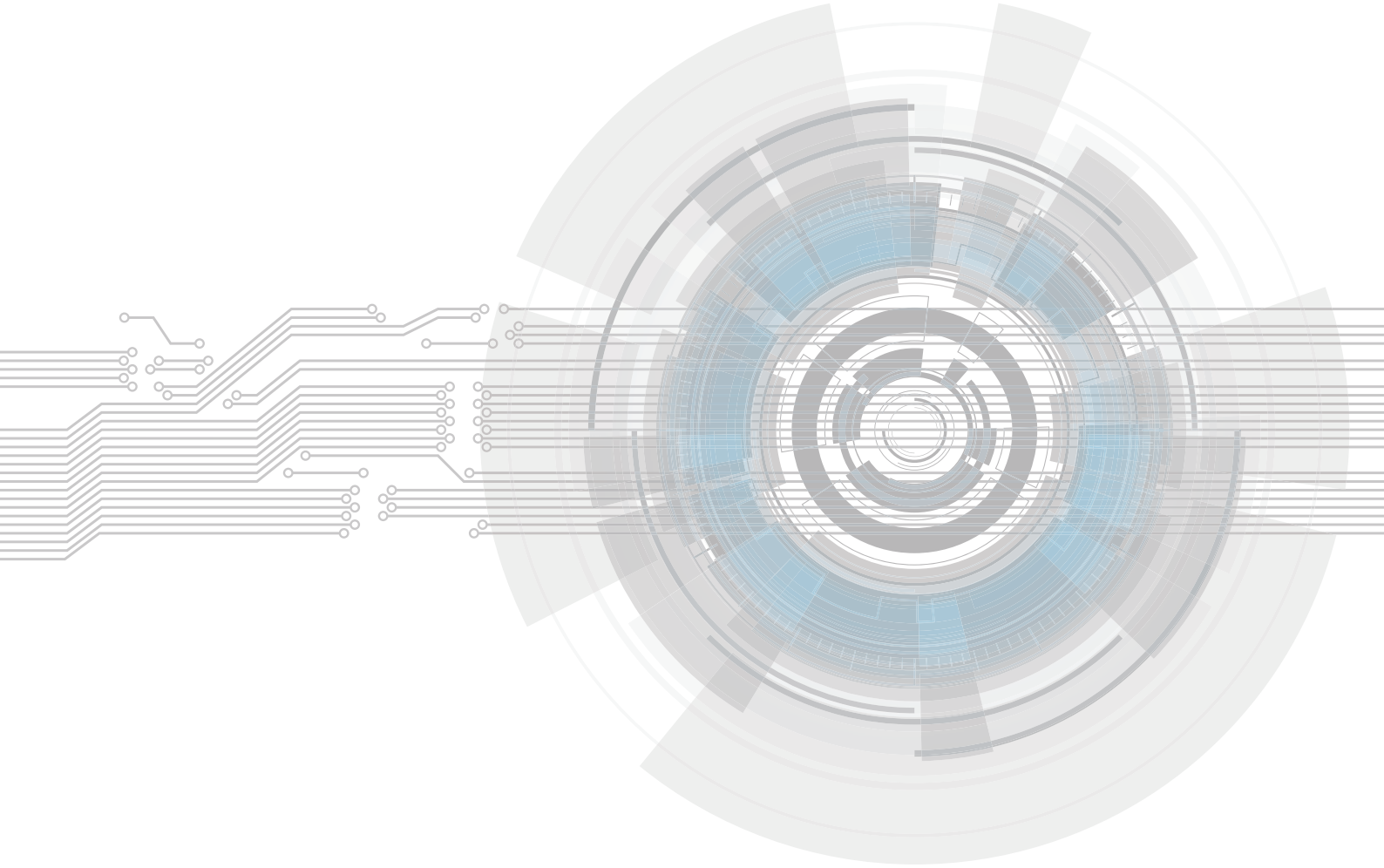
The fourth wave arrived after the HSMP visa regime ended in 2011. They usually worked for global companies with offices in London, at research organisations, or in education institutions. It is rare to find Russian start-up entrepreneurs in London, especially from the forth wave, since companies have to pay for their residence there. Just one case of a start-up entrepreneur emerged – an IT specialist who came to join a start-up team after long-term distant collaboration: *"when he [the founder] realises that he needs [you] right here and right now, and there are no possibilities to work remotely anymore, then efforts are made, like to certify organization to grant a visa…" (M, 26, Developer).*

These newcomers rarely sought communication with other Russians. They felt free to choose their own futures, and saw little need for the rituals and communities of the earlier arrivals. Most of them were integrated in company teams bearing a corporate identity and loyalty, and they did not limit themselves to local Russian communities. This generation moved from office to office within large global companies, and they went whenever the job it was located.

The sequential migration waves of Russian IT specialists each operated differently in the London IT market, which itself was dynamic and ever-changing. The first wave of IT émigrés to London in the late 1980s was composed mostly of academics, and its members quickly assimilated and developed a deep rootedness in local English life and everyday practices. The experience of these highly competent specialists established the basis for the "Russian techie" brand, although this reputation was not yet fully formed. With the collapse of the Soviet Union, migrants of the second wave of the 1990s became involved in speculation in the booming IT industry and pushed forward an authentic brand around the image of the "Russian techie" relying heavily on established network resources and the reputation of their predecessors. However, the final evolution of this brand only emerged during the third wave of the 2000s, which saw London as a point of attraction for Russians both because of a favourable immigration policy, and because a broad network of IT professionals with diverse communities had already gathered there. These people were at first able to exploit the already established the "Russian techie" brand to further their careers. But the arrival of some many new Russian émigrés, the brand was soon diluted and thus lost its cache. IT specialists crowded into temporary positions at banks as self-employed middle-range contract employees. Small professional communities turned into huge networks of new and barely familiar people. Identification of the Russian émigré as a unique and exceptional professional was transformed into a type of salaried short-term worker in large banks and corporations, a situation in which the status of "Russian techie" was no longer relevant or useful. As a reaction to these changes, some Russian professional communities began to erect entry barriers in order to retain their sense of elite status. Others dissolved and their members dispersed.

The case of the Russian IT specialists in London could have turned out differently than it did. It might have become a classics if story of "brain gain" (Rhode 1993, Meyer 2001), where immigration of qualified professionals takes place. It might also have been a happy story of "brain circulation" (Saxenian 2006) - returning these people's talents to Russia, enriching its IT culture and economy. But the rise and fall of the brand in British context means something else: it is barometer of conditions in Russia itself. The period of outflow, whose dynamics followed the twists and turns of developments in Russia, has ended, and the Russian professionals in London are moving on with their careers. But given current conditions, it is exceedingly unlikely that many will choose to bring their expertise back to their home country.

Because IT is the cutting edge of economic development around the world, Russia's position as a significant player on the global stage is dependent on the successful ecology of innovation in the IT sphere. Russian regions can conduct different experiments in IT development, but the recent trend toward "nationalization" of IT, or the policy of seeking "digital sovereignty" are moving the country in a direction which may well impede IT development and culture, for they threaten to cut the country off not only from the world economy, but also from those Russian IT professionals who might otherwise have returned. For example, at the moment of this writing, two families of my informants moved on to the USA and to Switzerland, several singles travelled to South-East Asia, and particularly Singapore – the seventh financial capital of the world. Only a few specialists have come back to Russia (Moscow) but mostly because of either visa problems or family issues. The brand of "The Russian Techie", which might have worked as a real trademark of the Russian IT professional worldwide and at home, and which could have placed Russia onto the map of global IT world, will likely now serve only to enrich the IT ecologies of other countries instead.



INFORMATION TECHNOLOGIES

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A study of approaches to reducing cost of ownership data warehouse exabyte sizes

SCIENTIFIC ORGANIZATION

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)

ABSTRACT

In this paper we present and compare four modern DFSs that are today widely used to deal with the problem of storage capacities and data access, federating the resource of distributed platform.

KEYWORDS

distributed file systems.

ACKNOWLEDGEMENTS

Andrianov E. A., Zaitsev K. S.

SUMMARY

Currently most of the market store data, including metadata, is a technology network storage NAS, for which reliable operation requires specialized, expensive equipment. An example of such equipment are widespread servers NetApp FAS8000, FAS2500 and other NetApp. Of course the establishment of data warehouse of a large company in this type of equipment will require significant financial resources.

In the last two or three years, rapidly evolving market for distributed file system having the properties of scalability to exabyte size, fault tolerance, reliability, and allows the user to deploy clusters on the cheap servers, which significantly reduces the cost of implementing data warehouses.

The report analyses the technical characteristics of the file systems (GlusterFS, Hadoop CephFS, MooseFS) at different loads and client-server configurations. For example, for the system Moose FS:

Possible protocols connection: FUSE

Test data transfer:

Configuration: 1 client / 1 server storage

File 1496 MB; time, 19 h; the speed of 78.6 MB/s

File 15394 MB; time 172 sec; speed 89.5 MB/s

Configuration 1 client / 2 server storage

File 1496 MB; time, 9 h; the speed of 166.6 MB/s

File 15394 MB; time 93 seconds; the speed of 165.5 Mbps

Configuration: 4 client (parallel recording) / 1 storage server

CLIENT1-File 1496 MB time 45 sec; the speed of 33.2 MB/s

Client2-File 1496 MB; time, 47 h; the speed of 31.8 MB/s

Client 3-File 1496 MB time 56 seconds; the speed of 26.7 MB/s

Client 4-File 1496 MB; time, 57 seconds; speed 26.2 MB/s

Configuration: 4 client (parallel entry) / 2 storage server

CLIENT1-File 1496 MB; time, 29 seconds; speed 51.6 MB/s

Client2-File 1496 MB time 34 sec; the speed of 44.0 MB/s

Client 3-File 1496 MB; time, 35 sec; speed 42.7 MB/s

Client 4-File 1496 MB; time, 33 h; the speed of 45.3 MB/s.

The results of the analysis demonstrate the possibility to scale the file system, issuing bandwidth, limited only by the speed of data transmission in the network. That in turn allows to refuse the use of expensive server hardware in favor of the distributed file systems.

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Simplified pilot module development and testing within the ATLAS PanDA Pilot 2.0 Project

SCIENTIFIC ORGANIZATION

Kurchatov Institute

ABSTRACT

To create a testing environment for module development and automated unit and functional testing for next generation pilot tasks, a simple pilot version was developed. It resembles the basic workflow of pilot tasks used in production and provides a simple and clean template for module construction. The miniPilot has a simple structure and is easy to use for development, testing and debugging server-client interactions with new protocols and application interfaces. The unit and functional test system will be developed on top of the miniPilot, and will be used to run automatic tests.

KEYWORDS

Workload management, development, testing.

ACKNOWLEDGEMENTS

On behalf of ATLAS collaboration.

SUMMARY

The Production and Distributed Analysis (PanDA) system has been developed to meet ATLAS production and analysis requirements for a data-driven workload management system capable of operating at the LHC data processing scale.

The PanDA pilot is one of the major components in the PanDA system. It runs on a worker node and takes care of setting up the environment, fetching and pushing data to storage, getting jobs from the PanDA server and executing them. The original PanDA Pilot was designed over 10 years ago and has since then grown organically. Large parts of the original pilot code base are now getting old and are difficult to maintain. Incremental changes and refactoring have been pushed to the limit, and the time is now right for a fresh start, informed by a decade of experience, with the PanDA Pilot 2.0 Project.

To create a testing environment for module development and automated unit and functional testing for next generation pilot tasks, a simple pilot version was developed. It resembles the basic workflow of pilot tasks used in production and provides a simple and clean template for module construction. The miniPilot has a simple structure and is easy to use for development, testing and debugging server-client interactions with new protocols and application interfaces. The unit and functional test system will be developed on top of the miniPilot, and will be used to run automatic tests.

This presentation will describe the miniPilot and the test system that will be used during the Pilot 2.0 Project.

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Graph Modification Problems: A modern perspective

SCIENTIFIC ORGANIZATION

University of Bergen

ABSTRACT

In network (or graph) modifications problem we have to modify (repair, improve, or adjust) a network to satisfy specific required properties while keeping the cost of the modification to the minimum. The commonly adapted mathematical model in the study of network problems is the graph modification problem. This is a fundamental unifying problem with a tremendous number of applications in various disciplines like machine learning, networking, sociology, data mining, computational biology, computer vision, and numerical analysis, and many others.

KEYWORDS

Algorithms, computational complexity, fixed-parameter tractability.

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dCache, managed Cloud Storage

SCIENTIFIC ORGANIZATION

DESY

ABSTRACT

For the previous decade, high performance, high capacity Open Source storage systems have been designed and implemented, accommodating the demanding needs of the LHC experiments. However, with the general move away from the concept of local computer centers, supporting their associated communities, towards large infrastructures, providing Cloud-like solutions to a large variety of different scientific groups, storage systems needed to adjust their capabilities in many areas. In this presentation we will elaboration on how those objects were achieved.

KEYWORDS

Cloud storage, big data, aai, protocols, webdav, cloud protocols, indigo-datacloud, qos.

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SUMMARY

For the previous decade, high performance, high capacity Open Source storage systems have been designed and implemented, accommodating the demanding needs of the LHC experiments. However, with the general move away from the concept of local computer centers, supporting their associated communities, towards large infrastructures, providing Cloud-like solutions to a large variety of different scientific groups, storage systems needed to adjust their capabilities in many areas, as there are federated identities, non authenticated delegation to portals or platforms, modern sharing and user defined Quality of Storage.

This presentation will give an overview on how dCache is keeping up with modern Cloud storage requirements by partnering with EU projects, which provide the necessary contact to a large set of Scientific Communities.

Regarding authentication, there is no strict relationship anymore between the individual scientist, the scientific community and the infrastructure, providing resourc-

es. Federated identity systems like SAML or “OpenID Connect” are growing into the method-of-choice for new scientific groups and are even sneaking their way into HEP. Therefor, under the umbrella of the INDIGO-DataCloud project, dCache is implementing those authentication mechanisms in addition to the already established ones, like username/password, Kerberos and X509 Certificates.

To simplify the use of dCache as back-end of scientific portals, dCache is experimenting with new anonymous delegation methods, like “Macaroons”, which the dCache team would like to introduce in order to start a discussion, targeting their broader acceptance in portals and at the level of service providers.

As the separation between managing scientific mass data and scientific semi-private data, like publications, is no longer strict, large data management systems are supposed to provide a simple interface to easily share data among individuals or groups. While some systems are offering that feature through web portals only, dCache will show that this can be provided uniquely for all protocols the system supports, including NFS and GridFTP.

Furthermore, in modern storage infrastructures, storage media, and consequently the quality and price of the request storage space are no longer negotiated with the responsible system administrators but dynamically selected by the end user or by automated computing platforms. The same is true for data migration between different qualities of storage. To accommodate this conceptual change, dCache is exposing it’s entire data management interface through a RESTful service and a graphical user interface. The implemented mechanisms are following the recommendation of the corresponding working groups in RDA and SNIA and are agreed-upon with the INDIGO-DataCloud project to be compatible with similar functionalities of other INDIGO provided storage systems.

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ATLAS Production System in heterogeneous computing environment

SCIENTIFIC ORGANIZATION

Kurchatov Institute

ABSTRACT

The new generation of the ATLAS production system is an automated workload manager, which used by thousands of physicists in CERN to process and analyze the distributed exabyte-scale data using the power of 150 computing centers, supercomputers and cloud academic resources. The system was developed in accordance with the requirements from ATLAS: high efficiency use of computing resources, automated load balancing and scalability. We present a description of the main elements of the system, their interactions and solutions used in the development of the system architecture.

KEYWORDS

Big Data; Grid-based Simulation and Computing; Parallel and Distributed Computing; Large Scale Scientific Instruments.

SUMMARY

The new generation of the ATLAS production system is an automated workload manager, which used by thousands of physicists in CERN to process and analyze the distributed exabyte-scale data using the power of 150 computing centers, supercomputers and cloud academic resources. The system was developed in accordance with the requirements from ATLAS scientific community: a flexible web user interface, fast adaptivity to new working processes, high efficiency use of computing resources, automated load balancing controlled by configurable policies for different types of data processing, scalability. It’s achieved through the use of a scalable multilevel system architecture. The high level interface for workflow management provides the abstraction of data and generates sets of input parameters - computing tasks based on user requests. These tasks are transferred to the executive low-level system to run in a heterogeneous computing environment. The task monitoring system provides continuous access to information about tasks

and necessary task management methods. We present a description of the main elements of the system, their interactions and solutions used in the development of the system architecture.

ADDITIONAL INFORMATION

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Tabu search heuristic for real-life vehicle routing problem

SCIENTIFIC ORGANIZATION

Higher School of Economics - National Research University

ABSTRACT

Vehicle Routing Problem is famous and popular problem in logistics and transportation, and the variety of such problems is explained by the fact that it occurs a lot in real-life situations. In this work, Site-Dependent Truck and Trailer Routing Problem with hard and soft Time Windows and Split Deliveries is considered (SDTTRPTWSD). Vehicle Routing Problem is NP-hard combinatorial optimization problem and finding an exact optimal solution is impossible. Tabu Search Heuristic is suggested as an algorithm for solving SDTTRPTWSD.

KEYWORDS

Vehicle Routing Problem, Tabu, Heuristic.

ACKNOWLEDGEMENTS

This work is partially supported by Laboratory of Algorithms and Technologies for Network Analysis, National Research University Higher School of Economics.

SUMMARY

The considered mathematical model is the same as in the article of Batsyn M., Ponomarenko A. (2014): Heuristic for a Real-life Truck and Trailer Routing Problem. However, the current work takes a different approach for program architecture is different. In this work, the program architecture for solving the Site-Dependent Truck and Trailer Routing Problem with hard and soft Time Windows and Split Deliveries (SDTTRPTWSD) problem is adapted for Heuristic with Tabu Search elements. Generally, it means that this architecture uses operations of deletion and insertion and both are evenly valued. Also, the algorithm employs greedy heuristic for initial solution; this greedy solution does not have a requriement to be obtained fast and to have a considerably good cost, because the heuristic with tabu elements is supposed to improve the initial solution significantly.

The base of the new algorithm is in two different representations of the route in program. First representation is Route Points, which are logical pieces of any route - every Route Point is a point that is visited by vehicle in this route. Second representation is Actions - atomic events such as travel from one point to another or process of unload at some point. By using these representations and intercation between them, the algorithm achieves the simplification and unification of the problem.

As for results, tests on real data show that the new algorithm architecture is capable of receiving a satisfactory results. In comparison with old architecture greedy algorithm, which is described in Batsyn M., Ponomarenko A. (2014), the costs for different real data days are generally improved by 5%. This number is substantial as it allows to save some real money for companies with such real problems. Also, there is an actual possibility to change the program in order to consider another TTRP or VRP problem or problem, which can be represented similarly.

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A Data Knowledge Base for Mega-Science Class Experiments Studies

SCIENTIFIC ORGANIZATION

Kurchatov Institute

ABSTRACT

Modern scientific research that requires integrated infrastructures, supports the entire lifecycle of the experiment, including the data processing chain, the software versioning management, description of the analysis algorithms, internal notes and the results published in scientific journals. Data Knowledge Base will be an infrastructure of such kind. It'll provide aggregation and integration of the miscellaneous and spreaded metadata sources within the ontological storage system, relevant to the specificity of experimental activities of the scientific communities.

KEYWORDS

Data knowledge base, ontology, experiment lifecycle, data analysis, data-intensive science, big data.

ACKNOWLEDGEMENTS

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SUMMARY

One of the main challenges of modern data-intensive science is the rapid increasing of the data volumes from experimental infrastructure and meta-information related to data processing and analysis, such as software releases, conditions data, information about data validity, etc. This problem is particularly relevant for the scientific research, ongoing and planned on the basis of the largest research facilities, such as the LHC, XFEL, NICA, ITER, FAIR, and others. In addition to the scientific data, these research complexes accumulate vast volumes of supporting meta-information describing all stages of the experimental studies life cycle. However, there is a lack of connectivity between the metadata describing the data processing cycle and the metadata representing the life cycle of scientific research in general, including annotation, indexing and publication of the results. As a consequence, it becomes boring and time consuming to reproduce scienific results - the most important criteria of the scientific knowledge truth.

It is difficult to estimate the problem of the scientific results verification. But the sampling results in some narrow areas, for example in the biomedical applications, show that the majority of research results published even in the lead academic journals can't be reproduced over time.

Laboratory of "Big Data" researchers have analysed the methods to store meta-information used by the ATLAS international collaboration at CERN. The task management system database stores meta-information about the computing tasks. Distributed Data Management database keeps the information of the data samples and controls the data transfer in a distributed computer environment. Internal notes, publications and conference proceedings are stored in the system of document circulation of CERN. Some meta-information is available in the form of Twiki pages and JIRA tickets. Listed storage systems are independent, information between them is loosely synchronized.

To verify the results in the ATLAS experiment, the researcher, guided by the data analysis, described in the publication, must identify data samples, based on which the research was conducted, as well as to reproduce the original state of hardware and software environment. Currently, this process is not automated and carried out manually due to the loose connectedness between data sources.

Proposed base of scientific knowledge will help to fill the existing gap in the holistic view of research lifecycle. In progress of the development the description of a scientific experiment in the ATLAS will be formalized, and the ontology will be developed. It will provide the connectivity between various sources of meta information.

Processing, synchronization and aggregation of data obtained from different metadata sources, including documentaries, will be implemented in a distributed repository (Hadoop). In the developed prototype of the knowledge base, this repository currently contains representational sample of ATLAS experiment metadata.

The annotation of scientific publications will be implemented using machine learning technologies, and a system of extracting information from documentary sources will be developed. This will allow us to get a software system that integrates data for physical experiments from different sources into a single ontological repository, and get all the information on the automated experiment in a coherent view.

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Machine Learning Technologies to Predict the ATLAS Production System Behaviour

SCIENTIFIC ORGANIZATION

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ABSTRACT

The ATLAS Production System (ProdSys2) is an automated scheduling system that is responsible for data processing, data analysis and Monte-Carlo production on the Grid, supercomputers and clouds. We proposed use of ML approach in conjunction with ProdSys2 jobs execution information to predict behavior of the system, starting with estimating task completion times. The WLCG ML R&D project was started in 2016, we will present our first results how ProdSys2 behavior could be predicted and simulated.

KEYWORDS

ProdSys, ATLAS, GRID, distributed computing, machine learning, anomaly detection.

ACKNOWLEDGEMENTS

This work was (in part) supported by Russian Governmental Program “Nauka”, N: 4.1661.2016.

SUMMARY

The second generation of the ATLAS Production System (ProdSys2) is an automated scheduling system that is responsible for data processing, data analysis and Monte-Carlo production on the Grid, supercomputers and clouds. The ProdSys2 project was started in 2014 and commissioned in 2015 (just before the LHC Run2) and now it handles O(2M) tasks per year, O(2M) jobs per day running on more than 250000 cores, each task transforms in many jobs. ProdSys2 evolves to accommodate a growing number of users and new requirements from the ATLAS Collaboration, Physics groups and individual users. ATLAS Distributed Computing in its current state is a big and heterogenous facilities, running on the WLCG, academic and commercial clouds and supercomputers. This cyber-infrastructure presents computing conditions in which contention for resources among high-priority data analyses happens routinely. Inevitably, over-utilized computing resources cause degradation of services or significant workload and data handling interruptions. For these and other reasons, grid data management and processing must inevitably tolerate a continuous stream of failures, errors, and faults. This makes simulating ProdSys2 behavior a very challenging task requiring unfeasibly large computing power. However, behavior of the system seems to contain regularities that can be modeled using Machine Learning (ML) algorithms. We proposed use of ML approach in conjunction with ProdSys2 jobs execution information to predict behavior of the system, starting with estimating task completion times. The WLCG ML R&D project was started in 2016, we will present our first results how ProdSys2 behavior could be predicted and simulated. On the next phase we will use ML algorithms to predict and to find anomalies in the ProdSys2 behaviour.

ADDITIONAL INFORMATION

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The Art of Femtosecond Laser Writing

SCIENTIFIC ORGANIZATION

University of Southampton and Mendeleyev University of Chemical Technology of Russia

ABSTRACT

Formation of sub-wavelength periodic structures in bulk transparent materials during irradiation with intense ultrashort light pulses remains a mystery. Nevertheless the phenomenon has enabled unique applications ranging from printed flat optics to eternal data storage.

KEYWORDS

Ultrafast laser material processing, Geometrical phase optics, Optical memory.

ACKNOWLEDGEMENTS

The work supported by the Ministry of Education and Science of the Russian Federation (Grant No. 14.Z50.31.0009) and the Engineering and Physical Sciences Research Council (EPSRC Project No. EP/M029042/1).

SUMMARY

Abstract: Formation of sub-wavelength periodic structures in bulk transparent materials during irradiation with intense ultrashort light pulses remains a mystery. Nevertheless the phenomenon has enabled unique applications ranging from printed flat optics to eternal data storage.

Modification of transparent materials with ultrafast lasers has recently attracted considerable interest due to new science and a wide range of applications ranging from 3D integrated optics and microfluidics to geometrical phase optics and durable data storage [1]. The key advantage of using femtosecond pulses for direct laser writing, as opposed to longer pulses, is that they can rapidly deposit energy in solids with high precision. The light is absorbed and the optical excitation ends before the surrounding lattice is perturbed, which results in highly localized nanostructuring without collateral material damage.

A decade ago it has been discovered the creation of sub-wavelength periodic structures with record small features of tens of nanometers self-organized along the polarization of light in the volume of silica glass, which is renowned for its high optical quality and chemical stability. On a macroscopic scale the self-assembled periodic nanostructure behaves as a uniaxial optical crystal with negative birefringence and slow axis oriented along nano-platelets of the structure. The optical anisotropy, which results from the alignment of the nano-platelets, referred to as form birefringence, is of the same order of magnitude as positive birefringence in crystalline quartz. More recently giant birefringence was also produced by ultrashort light pulses in amorphous hydrogenated silicon films [2].

A uniform birefringent layer can be imprinted by continuously scanning the material with a tightly focused laser beam. The control of the polarization orientation allows direct writing elements of flat optics with spatially variant anisotropy, which exploits Pancharatnam-Berry phase [3]. Unlike with refractive or diffractive elements the phase is not defined by optical path difference but results from the geometrical phase that accompanies space-variant polarization manipulation. The S-waveplate is one of the examples of such birefringent optical component, which can be used for producing optical vortexes and axially symmetric polarization states, e.g. radial or azimuthal, with applications ranging from optical trapping to microscopy and material processing [4, 5]. Another examples of the geometrical phase optical elements imprinted by ultrashort light pulses are Airy beam converters in silica glass (Fig. 1) and geometrical phase holograms in amorphous hydrogenated silicon (Fig. 2) The two independent parameters describing self-assembled form birefringence in quartz glass, the slow axis orientation (4^{th} dimension) and the strength of retardance (5^{th} dimension), were also explored for the optical encoding of information in addition to three spatial coordinates (Fig. 3). The slow axis orientation

and retardance were independently manipulated by the polarization and intensity of the femtosecond laser beam. The data optically encoded into five dimensions is successfully retrieved by quantitative birefringence measurements. The storage allows unprecedented parameters including hundreds of terabytes per disc data capacity and thermal stability up to 1000° [6]. Even at elevated temperatures of 190 °C, the extrapolated decay time of nanogratings is comparable with the age of the Universe - 13.8 billion years. The demonstrated recording of the first digital documents including the eternal copy of Newtons Opticks, which will survive the human race, is a vital step towards an eternal archive (Fig. 4). Also the projects such as Time Capsule to Mars (http://www.timecapsuletomars.com/) or Moon Mail (https://www.astrobotic.com/moon-mail) could benefit from the extreme durability of data imprinted by femtosecond laser in quartz glass, which is necessary for storage on Moon or Mars. The search of new materials and applications for ultrafast laser nanostructuring is currently in progress [7].

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ADDITIONAL INFORMATION

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Exabyte Scale Data Processing and Analysis System in Heterogeneous Computing Infrastructure

SCIENTIFIC ORGANIZATION

Kurchatov Institute

ABSTRACT

Exabyte Scale Data Processing and Analysis System in Heterogeneous Computing Infrastructure. The processing, management and analysis of data in the current Mega-Science-scale projects require integration of computing centers of different sizes, power and architecture into a single computing environment (cyberinfrastructure). When designing such an environment one must consider not only the disk and computing resources, but also the bandwidth of the global computing network and the throughputs and data access time between the computing centers.

KEYWORDS

BigData, LHC, NICA, Federated Storage, Workload Management System.

ACKNOWLEDGEMENTS

This work was funded in part by the Russian Ministry Education and Science award ГК №14.Z50.31.0024 . Many thanks to all our ATLAS and PanDA colleagues.

SUMMARY

Exabyte Scale Data Processing and Analysis System in Heterogeneous Computing Infrastructure.

“BigData Technologies for mega-science experiments” Laboratory, National Research Center “Kurchatov Institute”.

The Large Hadron Collider (LHC), operating at the international CERN Laboratory in Geneva, Switzerland, is leading Big Data driven scientific explorations. Experiments at the LHC explore the fundamental nature of matter and the basic forces that shape our universe, and were credited for the discovery of a Higgs boson. ATLAS, one of the largest collaborations ever assembled in the sciences, is at the forefront of research at the LHC. To address an unprecedented multi-petabyte data processing challenge, the ATLAS and other LHC experiments are relying on a heterogeneous distributed computational infrastructure.The ATLAS experiment uses PanDA (Production and Data Analysis Workload Management System) for managing the workflow for all data processing on hundreds of data centers. Through PanDA, ATLAS physicists see a single computing facility that enables rapid scientific breakthroughs for the experiment, even though the data centers are physically scattered all over the world. The scale is demonstrated by the following numbers: PanDA manages $O(10^2)$ sites, $O(10^5)$ cores, $O(10^8)$ jobs per year, $O(10^3)$ users and ATLAS Data Volume is $O(10^{17})$ bytes. In 2014 we started an ambitious program to expand PanDA to all available computing resources, including opportunistic use of commercial and academic clouds, supercomputers and Leadership Computing Facilities (LCF) to address LHC Run2 challenges. In 2015 the Large Hadron Collider opened new “Gates of Nature” by reaching instantaneous luminosities exceeding 2·1034 cm-2 s-1 and center of mass energies of 13 TeV. The physics goals of the the experiments include searches for physics beyond the Standard Model and high precision Higgs sector studies. These goals require detailed comparison of the expected physics and detector behavior with data. As of today ATLAS manages more than 200 petabytes of data on more than hundred computational sites.

We’ve developed, deployed and operating the next generation of the ATLAS Production System to deal with widely distributed data volume and to do data processing on heterogeneous computing environment. The system has unique characteristics and its operates on 250 000 computing cores and more than 1.3 exabytes have been processed in 2015.

Another important research topic is building a federated computing infrastructure. Aristotle asserted that “the whole is greater than the sum of its parts”, so the integration of heterogeneous computing centers into a single federated distributed cyberinfrastructure allows more efficient utilization of computing and disk resources for a wide range of scientific applications. To address it in 2015 in the framework

of the Laboratory “Big Data Technologies for mega-science class projects” in NRC “Kurchatov Institute” a work has begun on the creation of a united disk resource federation for geographically distributed data centers, located in Moscow, St. Petersburg, Dubna, Gatchina and CERN (Geneva), its integration with existing computing resources and provision of access to this resources for applications running on both supercomputers and high throughput distributed computing systems. It was demonstrated that such cyberinfrastructure can be efficiently used for data processing and analysis by the LHC scientific applications, as well as for bioinformatical applications.

Klyunin Alexey
Engineer

Human-Free Robotic Automation of Industrial Operations

SCIENTIFIC ORGANIZATION

ITMO University

ABSTRACT

This paper is a result of the university-industry collaboration between ITMO University and Thermex. A subject of this cooperative investigation is robotic automation of industrial operations in the sense of organizing a cyber-physical system and eliminating the human factor from the production. Tasks of a technological process considered in the paper are welding, transporting and polishing. They are simulated on the basis of the laboratory of the Department of Control Systems and Informatics. Robots used in this study are Mitsubishi MELFA RV-3SDB, KUKA youBot and Kawasaki FS06N.

KEYWORDS

Robots, industry, manipulators, automatic factory.

ACKNOWLEDGEMENTS

This paper is supported by Government of Russian Federation (GOSZADANIE 2014/190 (project 2118)), the Russian Federation President Grant №14. Y31.16.9281-НШ and the Ministry of Education and Science of Russian Federation (project 14.Z50.31.0031).

ADDITIONAL INFORMATION

Oleg I. Borisov, Vladislav S. Gromov, Sergey A. Kolyubin, Anton A. Pyrkin, Alexey A. Bobtsov, Vladimir I. Salikhov, Alexey O. Klyunin and Igor V. Petranevsky.

Korchuganova Tatiana
Specialist degree
Design engineer

ATLAS BigPanDA Monitoring and Its Evolution

SCIENTIFIC ORGANIZATION

Tomsk Polytechnic University

ABSTRACT

BigPanDA is the latest generation of the monitoring system for the Production and Distributed Analysis (PanDA) system. The BigPanDA monitor is a core component of PanDA and also serves the monitoring needs of the new ATLAS Production System Prodsys-2. BigPanDA has been developed to serve the growing computation needs of the ATLAS Experiment and the wider applications of PanDA beyond ATLAS.

KEYWORDS

ATLAS production and distributed analysis, monitoring system, disributed computing.

SUMMARY

BigPanDA is the latest generation of the monitoring system for the Production and Distributed Analysis (PanDA) system. The BigPanDA monitor is a core component of PanDA and also serves the monitoring needs of the new ATLAS Production System Prodsys-2. BigPanDA has been developed to serve the growing computation needs of the ATLAS Experiment and the wider applications of PanDA beyond ATLAS. Through a system-wide job database, the BigPanDA monitor provides a comprehensive and coherent view of the tasks and jobs executed by the system, from high level summaries to detailed drill-down job diagnostics. The system has been in production and has remained in continuous development since mid 2014, today effectively managing more than 2 million jobs per day distributed over 150 computing centers worldwide. BigPanDA also delivers web-based analytics and system state views to groups of users including distributed computing systems operators, shifters, physicist end-users, computing managers and accounting services. Providing this information at different levels of abstraction and in real time has required solving several design problems described in this work. We describe our approach, design, experience and future plans in developing and operating BigPanDA monitoring.

ADDITIONAL INFORMATION

Co-authors: Siarhei Padolski (Brookhaven National Laboratory) Torre Wenaus (Brookhaven National Laboratory)

Korenkov Vladimir

Doctor of technical Sciences

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Trends in the development of distributed computing and Big data technologies to support mega-projects

SCIENTIFIC ORGANIZATION

Joint Institute for Nuclear Research (JINR)

ABSTRACT

The experiments at the Large Hadron Collider (LHC) at CERN (Geneva, Switzerland) played a leading role in scientific research. Processing and analysis of data is carried out using GRID systems, academic, national and commercial resources of cloud computing, supercomputers and other resources. For large mega-projects in Russia (for example, NICA at JINR) creates a heterogeneous distributed computer environment, based on the trends of development of information technologies.

KEYWORDS

Distributed computing, Big data, grid, cloud, HPC.

SUMMARY

Distributed infrastructure for data processing and analysis of the experiments at the Large hadron Collider and the evolution of their development presented in the report. Problems of integration of different distributed computing architectures (grid, cloud, HPC) are analyzed on the basis of the experience of participation in many large-scale projects. Simulation of computer infrastructure for the mega-project of NICA held on the basis of parameters of the physical detectors and data processing scenarios. Computer infrastructure mega-project is developed on the basis of trends of development of information technologies.

Krasnopevtsev Dimitrii
Engineer researcher

Study of ATLAS Transition Radiation Tracker performance with supercomputers and federated data storage system

SCIENTIFIC ORGANIZATION

Kurchatov Institute

ABSTRACT

One of the most important studies dedicated to be solved for ATLAS physics researches is a reconstruction of proton-proton events with large number of interactions in the Transition Radiation Tracker (TRT). This study includes TRT performance results obtained with the usage of the standard ATLAS GRID as well as Kurchatov Institute's supercomputer and federated data storage system based on resources of NRC KI, PNPI and SPbSU Universities. In addition to a physics results the analysis of CPU efficiency during these studies is presented.

KEYWORDS

ATLAS, supercomputer, transition radiation tracker, TRT.

SUMMARY

After the early success in discovering a new particle consistent with the long awaited Higgs boson, the Large Hadron Collider (LHC) experiments have started the precision measurements and they are ready for further discoveries that will be made possible by much higher LHC collision rates during Run 2. ATLAS, one of the four experiments at the LHC, is leading a computing evolution program to evolve their software and computing model to make the best possible usage of available resources, including supercomputers. A proper understanding of the detectors performances at high occupancy condition is important for many on-going physics analyses. The ATLAS Transition Radiation Tracker (TRT) is one of these detectors.

TRT is a large straw tube tracking system that is the outermost of the three subsystems of the ATLAS Inner Detector (ID). TRT contributes significantly to the resolution for high-pT tracks in the ID providing excellent particle identification capabilities and electron-pion separation. ATLAS experiment is using Worldwide LHC Computing system (WLCG) GRID. WLCG is a global collaboration of computer centers and it provides seamless access to computing resources, which include data storage capacity, processing power, sensors, visualization tools and more. WLCG resources are fully utilized and it is important to integrate opportunistic computing resources such as supercomputers and federated data storage systems not to curtail the range and precision of physics studies.

One of the most important studies to be solved for ATLAS physics researches is the reconstruction of proton-proton events with large number of interactions in TRT. It becomes clear that high-performance computing contributions become important and valuable. An example of a very successful approach is National Research Centre Kurchatov Institute's (NRC KI) Data Processing Center including Tier-1 GRID site, supercomputer and at the same time linked to the federated storage system.

The presented studies include TRT performance results obtained with the usage of the standard ATLAS GRID as well as Kurchatov Institute's supercomputer and federated data storage system based on resources of NRC KI, Petersburg Nuclear Physics Institute and St.-Petersburg State University. In addition to a physics results the analysis of CPU efficiency during these studies is presented.

Lassnig Mario
Doctor of Natural Sciences
Staff Scientist

Data Management For Exascale Experiments

SCIENTIFIC ORGANIZATION

European Organization for Nuclear Research (CERN)

ABSTRACT

The High-Energy Physics Experiment ATLAS has processed more than an Exabyte of data during its operation, and is growing continuously. In this talk, I present the solutions we developed for the data management system that serves as the foundation for ATLAS. First, I give an overview of the global requirements. Then I present selected highlights, specifically (a) how we dynamically schedule competing requests over constrained storage and network, (b) how we deal with with data loss and recovery, and (c) how we dynamically adapt our data placement based on the analysis of system usage.

KEYWORDS

Data management, distributed systems, databases, networks, analytics.

ACKNOWLEDGEMENTS

This work has been carried out within the ATLAS Experiment, which consists of 38 member states and more than 170 institutes worldwide. I am also deeply grateful to Prof. Alexei Klimentov for the support and opportunity to present our work at this conference.

SUMMARY

Part 1 - Introduction

- The ATLAS Experiment
- Workflow and Data Management

Part 2 - Data Management

- Requirements from workflow management
- Declarative data management with rules and subscriptions
- Global infrastructure and system operations

Part 3 - Highlights

- Request scheduling for transfer and deletion
- Data loss and recovery
- Smart placement using data access patterns
- System analytics: How we keep track of everything

Part 4 - Outlook and Summary

- Data management evolution: The challenge of serving single events
- Conclusions

ADDITIONAL INFORMATION

Invited speaker on behalf of Prof. Alexey V. Kavokin and Prof. Alexei Klimentov.

Nikolaev Alexey
Master
Probationer

Algorithm Selection for the Maximum Clique Problem

SCIENTIFIC ORGANIZATION

Laboratory of Algorithms and Technologies for Network Analysis

ABSTRACT

In this talk a new approach for solving the maximum clique problem is presented. For every instance the suggested approach predicts if a heuristic should be used before starting an exact algorithm and predicts the fastest algorithm from several algorithms for the maximum clique problem. Then the chosen algorithm is applied for solving the maximum clique problem in a given graph. According to the computational results the proposed approach is effective and it overcomes state-of-the-art exact algorithms.

KEYWORDS

Maximum clique problem, exact algorithms, machine learning.

ACKNOWLEDGEMENTS

This work is supported by Laboratory of Algorithms and Technologies for Network Analysis, National Research University Higher School of Economics.

SUMMARY

A simple, undirected graph G = (V ,E) is defined by a set of vertices V = {v1, v2,...,vn} and a set of edges E made up of pairs of distinct vertices ($E \subseteq V \times V$). A clique in graph G is a complete subgraph, that is, a subgraph in which vertices are pairwise adjacent. In this work, we consider the maximum clique problem (MCP), which asks for a clique of the largest cardinality in the graph. The size of a maximum clique is called the clique number of the graph and is usually denoted as ω(G).

The MCP is a well known and deeply studied NP-hard problem in graph theory. Moreover, it has found applications in many different fields, such as data association problems in bioinformatics and computational biology [1–3], computer vision [4], and robotics [5]. Such association problems may be reduced to the MCP in a correspondence graph, which subsumes the matching criteria between the two entities involved. With the upsurge of Web technologies, cliques have also been applied to capture the structure of massive networks. For example, in social networks a clique can identify a group of cooperating agents (e.g. a terrorist cell); in the World Wide Web, cliques or quasi-cliques can help detect frequently visited pages concerning a certain topic. Clique kernels can also help to identify clusters.

In the literature, there are many different approaches to solving the MCP exactly. Most successful exact solvers belong to the family of branch-and-bound algorithms that employ approximate-colour bounds [6–12]. But theoretical analysis of these algorithms appears to be difficult. Instead of it empirical analysis of the algorithm properties is made using DIMACS benchmarks. Many papers on this topic conclude that a new algorithm is better than other algorithms, if it spends less time in total on solving benchmarks than other algorithms. However the fact that some specific algorithms turn out to show better results for some specific graphs is usually ignored.

The ideal solution for this problem is to create a kind of “oracle” algorithm that would predict how much time each of the existing algorithms would spend on solving the MCP for a given graph. After that the oracle would choose the fastest algorithm. Unfortunately there is no such thing as the ideal oracle thus in practice we can only develop a heuristic for predicting the fastest algorithm from a predifined set of exact algorithms.

This work presents an approach which is based on machine learning. It selects the fastest algorithm from the set of state-of-the-art solvers. In order to do it some features were extracted and are used for the proposed approach. The computational results show that the suggested aproach is effective.

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ADDITIONAL INFORMATION

Joint work with Denis Kirisov, Mikhail Batsyn, Pablo San Segundo.

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Doctor of science

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SCIENTIFIC ORGANIZATION

Joint Institute for Nuclear Research

Data intensive Science in HEP

ABSTRACT

Experimental High Energy Physics demands two main issues: (1) the giant complexes for distributed computing and corresponding grid-cloud internet services as WLCG; (2) Machine Learning approaches to search for unevident regularities in data for getting the most probable forecast of phenomena under study. Both issues are considered on examples of the JINR practice.

KEYWORDS

Data intensive science, grid-cloud services, machine learning, simulation, neural networks, clustering.

SUMMARY

The new challenging era of scientific data management in the coming decade of “Big Data” requires a new paradigm named data intensive science to deal with

Exabyte data scale in many modern social, economic and scientific areas. Experimental High Energy Physics, in particular, demands two main issues: (1) the giant complexes for distributed computing and corresponding grid-cloud internet services as the Worldwide LHC Computing Grid (WLCG); (2) Machine Learning (ML) approaches to search for unevident regularities in data for getting the most probable forecast of phenomena under study. The first issue is considered on examples of the grid/cloud systems developed at the Laboratory of Information Technologies (JINR, Dubna) and focused on improving their development efficiency. For this purpose a simulation program is proposed which is designed to use work quality indicators of some real system to design and predict its evolution. The second issue is also considered on examples of such ML applications in the JINR practice as artificial neural networks, two stage clustering and some others.

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Output Robust Control with Anti-Windup Compensation for Robotic Boat

SCIENTIFIC ORGANIZATION

ITMO University

ABSTRACT

In this work a problem of saturated control for a robotic boat with unknown parameters and unmeasurable velocity and acceleration is addressed. The controller design is based on the output robust control approach “consecutive compensator” augmented with an integral loop, which allows to eliminate a static error and implement the anti-windup scheme. As result, the regulator generating the bounded control signal and avoiding windup was obtained. The efficiency of the proposed algorithm was illustrated by the experimental approval using the robotic boat setup.

KEYWORDS

Robotics, Output control, Robust control, Anti-Windup.

ACKNOWLEDGEMENTS

This paper is supported by Government of Russian Federation (GOSZADANIE 2014/190 (project 2118), subsidy 074 -U01, project 14.Z50.31.0031).

SUMMARY

In this paper a problem of saturated control for a robotic boat with unknown parameters and unmeasurable velocity and acceleration is addressed. The controller design is based on the output robust control approach ``consecutive compensator”. It was augmented with an integral loop, which allows to eliminate a static error and implement the anti-windup scheme to reduce overshoot of the output variable. As result, the regulator generating the bounded control signal and avoiding windup for the boat was obtained. The efficiency of the proposed algorithm was illustrated by the experimental approval using the robotic boat setup. The comparison between three types of controllers (regular consecutive compensator, integral modification and one equipped with anti-windup) is presented.

This practical study is devoted to development of simple control algorithms, which can be useful in stabilization tasks of various applications. The proposed in this paper robust output controller with anti-windup compensation has shown the satisfactory experimental results at the robotic boat setup. This approach is applicable for plants with bounded input and uncertain parameters. Its useful feature is a possibility to specify limits of the generated control signal with reduced (or even without) undesirable overshoot of the output variable. It is important for real technical systems due to their hardware constraints

The results of the experiments are presented in Figs.~\ref{experimental_approval_inputs} and \ref{experimental_approval_error}. Note that these plots correspond only to motion along X-axis. The original and saturated control signals generated by the consecutive compensator with anti-windup are depicted in Fig.~\ref{experimental_approval_inputs}. Three plots of the output variable are illustrated

in Fig.~\ref{experimental_approval_error}. The green curve is assigned to the regular consecutive compensator (\ref{regular_control_law_experiment}), the blue one corresponds to the integral consecutive compensator (\ref{integral_control_law_experiment}) and the last red curve refers to the consecutive compensator equipped with the anti-windup scheme (\ref{control_law_AW_experiment}). The process of motion and visualization of the computer vision are shown in Fig.~\ref{experiment}. As it can be seen on the obtained plots the regular consecutive compensator leads to the small static error caused by the nonlinear input of the actuators. Small values of error lead to small control, which is not sufficient to counteract waves and move the boat. This effect is removed by the integral term, which accumulates the error value and increase the control signal. Note that increasing of the controller parameters is undesirable, because it may lead to self-oscillations of the boat. Smooth red curve is achieved by the anti-windup approach. Little oscillations of the boat are caused by wave disturbances and noise in the measurement channels.

Ponomarenko Alexander
Master Degree
Research Fellow

Algorithms for building highly scalable distributed data storages

SCIENTIFIC ORGANIZATION

National Research University
Higher School of Economics

ABSTRACT

One of possible ways to implement highly scalable data storage is to build a structured P2P network. This approach has been successfully used in DHT systems. However the search in DHT systems is restricted by the search of exact hash values. This makes it impossible to build data storages that can efficiently perform complex queries. In this talk we will discus a class of algorithms, which overcomes this limitations and can be used as a basis for building highly scalable distributed storages with the ability to efficiently perform similarity search in metric and semimetric spaces.

KEYWORDS

Algorithms, peer-to-peer, scalability, data storages, distributed systems, nearest neighbour search, similarity search, metric space.

ACKNOWLEDGEMENTS

This work is partially supported by Laboratory of Algorithms and Technologies for Network Analysis, National Research University Higher School of Economics.

SUMMARY

The ability to scale is a desirable business requirement for computer systems. Data storage is a central part of any computer system. The scalability of any computer system strongly depends on the ability to scale of its data storage. One of possible ways to implement highly scalable data storage is to build a structured P2P network on the level of data or on the level of physical nodes. This approach has been successfully used in well-known DHT systems, which can be considered as distributed key-value storages. However the search in DHT systems is restricted by the search of exact hash values. This makes it impossible to build data storages that can efficiently perform complex queries. In this talk we will discus a class of algorithms, which overcomes this limitations and can be used as a basis for building highly scalable distributed storages with the ability to efficiently perform similarity search in metric and semimetric spaces.

ADDITIONAL INFORMATION

Winner of Ilya Segalovich scholarship by Yandex Winner of IBM PHD Student scholarship award.

Poyda Alexey
PhD
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The ATLAS PanDA Workload Management System Evaluation For Genome Sequencing Data Analysis On NRC "Kurchatov Institute" Computing Facilities

SCIENTIFIC ORGANIZATION

Kurchatov Institute

ABSTRACT

In this paper we will describe our recent accomplishments how bioinformatics application can be run by PanDA Workload Management System on supercomputers and clouds.

KEYWORDS

Workload management system, genome sequencing data analysis, supercomputers.

ACKNOWLEDGEMENTS

This work was funded in part by the Russian Ministry of Science and Education under Contract No 14.Z50.31.0024 and by RFBR according to the research project №16-37-00249 mol_a. This work was carried out using high-performance computing resources of federal center for collective usage at NRC "Kurchatov Institute", http://computing.kiae.ru/. We wish to thank all our colleagues who contributed to PanDA evaluation at NRC KI and especially PanDA core SW team.

SUMMARY

Modern biology operates with a large amount of data and investigates very complex systems. Scientists use complicated algorithms and very sophisticated software, which is impossible to run, without access to significant computing resources. In addition, modern biology requires efficient large data volumes processing, such as DNA sequences, proteins structure, Genome Scale Modeling, and molecular dynamics simulation. Recent advances in Next Generation Genome Sequencing technology led to significant increase in amount of sequencing data that has to be processed, analysed and made available for bioinformaticians worldwide. The ancient DNA analysis is one of the most challenging and CPU consuming scientific problems.

It can take a couple of months on super-computer at NRC KI to run widely used package PALEOMIX to analyse ancient genome sequencing data. The issue of data processing at a large scale has been addressed in the past by the LHC experiments at CERN and in our studies we have evaluated and adapted Workload Management System (WMS) PanDA initially developed and deployed by the ATLAS experiment for the LHC data processing and analysis. To improve the PALEOMIX workflow performance we split input data into chunks to process them simultaneously and at the end transient results are merged. The above scenario allowed us to run many parallel tasks on the distributed computing resources (supercomputer and academic cloud) at the NRC "Kurchatov Institute".

The dedicated PanDA instance has been installed, adapted and used at NRC KI to define and to broker data processing tasks to available computing resources. PanDA also managed tasks execution during the whole payload life cycle. It dramatically decreased the total walltime, in comparison with the traditional monolithic workflow execution. Task execution time was reduced from several weeks to several days, and it was demonstrated for Mammoths DNA samples analysis.

In this paper we will describe our recent accomplishments how bioinformatics application can be run by PanDA Workload Management System on supercomputers and clouds.

Schulz Markus
PhD
Senior Researcher

The World Wide LHC Grid (WLCG), a large scale distributed scientific computing infrastructure

SCIENTIFIC ORGANIZATION

CERN Geneva, Switzerland

ABSTRACT

WLCG, a federation of more than 170 computer centres in 42 countries, provides since 2008 the computing and storage required by the experiments of the LHC accelerators. It gives more than 10000 physicists seamless access to 300 PBytes and more than 600.000 cores. The lecture will describe the technology, operation and the evolution of this system.

KEYWORDS

Distributed computing, scientific computing, grid computing, cloud computing.

Spokoiny Vladimir
Prof.
Prof., Head of research group

Adaptive Weights Clustering

SCIENTIFIC ORGANIZATION

Skoltech, MIPT, WIAS and HU Berlin

ABSTRACT

This paper presents a new non-parametric method of cluster analysis called Adaptive Weights Clustering. The proposed procedure aims at describing the clustering structure in terms of weights w_{ij} which is computed from the data by an iterative procedure. The method is fully adaptive and does not require to specify the number of clusters or their structure. The procedure is able to recover different clusters with sharp edges or manifold structure. A numerical study illustrates a nice performance of the method.

KEYWORDS

Cluster gap, propagation, separation.

Utkina Irina
Bachelor
Student

Optimal graph for decentralized search problem

SCIENTIFIC ORGANIZATION

Higher School of Economics - National Research University

ABSTRACT

One of the approaches for the nearest neighbor search problem is to build a network which nodes correspond to the given set of indexed objects. In this case the search of the closest object can be thought as a search of a node in a network. A procedure in the network is called decentralized if it uses only local information about visited nodes and its neighbours. Several algorithms that construct such networks have been proposed in literature. We propose a programming model and tabu algorithm for constructing network.

KEYWORDS

Networks, tabu, heuristic, search.

ACKNOWLEDGEMENTS

This work is partially supported by Laboratory of Algorithms and Technologies for Network Analysis, National Research University Higher School of Economics.

SUMMARY

One of the approaches for the nearest neighbor search problem is to build a network which nodes correspond to the given set of indexed objects. In this case the search of the closest object can be thought as a search of a node in a network. A procedure in the network is called decentralized if it uses only local information about visited nodes and its neighbors. Networks, which structure allows efficiently performing the nearest neighbor search by a decentralized search procedure started from any node, are of particular interest especially for pure distributed systems. Several algorithms that construct such networks have been proposed in literature. However, the following questions arise: “Are there network models in which decentralized search can be performed faster?”; “What are the optimal networks for the decentralized search?”; “What are their properties?”. In this talk we partially give the answers to these questions. We propose a programming model for the problem of determining an optimal network structure for decentralized nearest neighbor search. Also we propose tabu algorithm for constracting such networks and show results.

Vorobyev Daniil

Master

Engineer

Software system for data processing

SCIENTIFIC ORGANIZATION

National University of Science and Technology «MISIS»

ABSTRACT

Technical solutions are suggested for structure, functions and organization of data processing tools based on WEB technology systems and cloud resources. We formulate the strategic direction of the development of a software system fo higher-performance processing of large volumes of electronic data for the problems of intellectual structural analysis: classification, machine learning and prognostication in quantum physics.

KEYWORDS

Big data, neural network, data mining, data base, VASP.

SUMMARY

Today is the day we can say that over the past decades have seen intensive development of automated information systems (AIS), including in areas such as network technology Internet ways of storing and representing knowledge, programming languages and tools, artificial intelligence techniques, algorithms, distributed and cloud computing etc.

Scientific and technical achievements in the field of artificial intelligence influenced the formation of new and transformation of the old classes of information systems -. Intelligent information systems, data mining, expert systems, decision support systems, etc. Unfortunately, all modern tools in most cases scattered, decide chastnopredmetnye task or development “of the system” that integrates in its structure all of the most advanced tools (approaches, striving to improve the efficiency of the use of information stored in electronic form.

Specificity IDPSimposes a significant imprint on the methodology and technology of its development. Technology for creating IDPShas its essential features and is different from the design and development process each information and software systems. These differences are to a large extent determined by the fact that Gozo is an intelligent information systems (MIS) based on the ideas, principles and techniques of artificial intelligence (AI). Such systems require for their realization the specialized approaches, methods and technologies are largely different from the classical methods of software development sisge However, the ever-increasing interest in artificial intelligence contributes to more widespread adoption and use of intelligent systems in different application areas. The development of artificial intelligence systems (expert-oriented systems, data mining systems, translation, machine vision t i. E.) Is gradually coming to an industrial scale, it acquires industry features. This leads to the fact that such systems are beginning to be brought to the same requirements as the traditional program products. Specificity of Gozo lies in the fact that the development and implementation of intelligent information systems rather long and

laborious process, which has not yet been fully worked out, and often requires new efficiency and quality of the resulting system is largely determined by the talent and expertise of its developers. In addition, the problem of implementation is also connected with the choice of appropriate means of development, which is a separate challenge. Modern analytical information systems acquire the characteristics and features of software systems, based on data mining algorithms, expert systems, artificial intelligence systems, and machine learning. We single out the following basic features IDPS, defining it as a tool for expert support

- Ability to solve a wide range of tasks in a formalized problem area.

- The ability to extract knowledge published and present them in the form of formal models of knowledge.

- Modeling of intellectual property rights mechanisms.

- The use of domain knowledge.

- The use of heuristic methods for solving problems.

- Ability to explain the decision.

- High performance. Etc.

cloud computing technology. Cloud computing is called a complex based on virtual machines, capable of a minimum of delay, on demand, to increase or decrease its performance.

Remote computing service cloud can be called, if it satisfies the regulations formed the American NITS (National Institute of Standards and Technology) (Standards Acceleration to Jumpstart Adoption of Cloud Computing (SAJACC). All provided cloud services divide into three basic

- Infrastructure as a service - infrastructure as a service. The user is given an unlimited set of virtual machines whose configuration configures the user, the user is also able to bind them to the network and thus to build a virtual cluster of the configuration that he needs. At this level, the user has no control over the iron only, everything else is subject to it.

- Platform as a service - platform as a service. The level where the user is abstracted from the level of virtual machines, networks, clusters. At this level, the user as it has at its disposal an infinite size disk, the computer with infinite memory and super-fast multi-core processor. In fact, the platform is constructed so that organizes cluster that looks like a single machine.

- Software as a service - Software as a Service. Users remotely using any program. There is a cloud version of 1C, Photoshop, offisnyh programs. User configuration is available only to its account in proramma and configuration of the program in its session.

Data Mining Platform. The developed platform can refer to a category of SaaS

The system also includes client-side extension functionality, and it is expected that the system will have a part of the PaaS functionality.

The developed platform has the following features (SaaS BI):

- As service is available workspace (authentication and authorization means download and edit files).

- A library of algorithms and analysis subsystems, including: clustering and classification, the construction rules and decision trees, neural networks, genetic algorithms, statistical algorithms, and so forth..

- Means of construction of automatic collective solutions based on algorithms.

- Analysis of the effectiveness of training tools on the data.

- Visualization of analysis results.

By strategic plans include the possibility of expanding user features for the creation and adjustment of individual sections of the library of algorithms (PaaS), including:

- Editor to generate new algorithms based on the meta-language.

- Ability to upload algorithms to public access.

- Ability to build scripts using analysis algorithms.

- Integration with business processes of users / customers (the server automatically at the end of the analysis or training will be specifically configured to send data to the customer's server and thus will

- Work with the server via the API (automatic data entry in Gozo).

Strategic development plan. intelligent data processing system (IDPS) is a software and hardware system, configured to use different classes of recognition, language and focused on providing services in the field of scientific and applied problems of a variety of processing.

The complex integrates incorporates a high-performance hardware (including high performance computing servers and extensive disk storage) and efficient software (software) designed for a wide range of applications of data mining and permitting the setting and the expansion of supported features.

The system supports and implements the concept of "public cloud computing» (public cloud computing) and offers the following categories of the "cloud" services:

- Software as a service (Software as a Service, SaaS) - users of the system through the Internet access g specialized software and a web interface that runs in any modern browser, have the opportunity to use it to solve their problems, including resource-intensive;

- Infrastructure as a service (Infrastructure as a Service, IaaS) - users of the system can be rented for long term resources of a computer infrastructure when needed, such as computing servers and storage systems, as well as to attract to solve their problems intellectual resources provided by the staff, providing support to the functioning and development of the system.

IDPS main functions:

- The system provides a means for solving the problems of the following areas: statistical data processing (correlation and regression analysis of variance and covariance analysis, etc...), Pattern recognition (classification with training), clustering (classification without training), identification (identification of distinctive signs of the objects), forecasting (the definition of tendencies of development process of extracting knowledge published (data mining) and text (text mining). The open architecture and API system set of supported classes of problems can be simply amended, including by the use of the decisive third-party modules developers.

also HTML, from a spreadsheet in Excel and the OpenDocument format, from relational databases, as well as from veb¬prilozheny and services, such as Google spreadsheets, databases or Zoho Creator Yandex service. Furthermore m th data can be entered, modified and edited directly through the system interface. Export of data and may be in different file formats, in particular, CSV, XML, HTML, PDF. RTF, Excel JPEG, PNG. In addition to these, the system can be integrated into other converters imporga / eksporga providing work with specific formats and data sources.

- IDPScontains tools that provide opportunities for visualization and graphical representation of the original data and the results of their processing in various forms, including in the form of all sorts of graphs and charts, as well as to generate a variety of reports that can be published as part of the system or exported for later use outside IDPS.

- The system includes interactive tutorials, guides and test modules on the subject of intellectual data processing designed to educate users effectively address the relevant problems through the system, as well as to increase their level of knowledge about the models and methods of data processing. In addition, the SIS provides opportunities for the organization on the basis of its e-learning courses and conduct automated testing knowledge of different subject areas.

- For each user IDPS automatically creates a website that functions within the system and available to other users. On its Web site, the user can aggregate and publish any materials that do not contradict the rules adopted in the system, and limit access to them when needed. In addition to the content, the users within a certain range can change the design and structure of their sites.

- The system supports a variety of communication services for communication between a user and receive feedback from them, which may include the exchange of electronic messages (including chat in real-time) and mailing lists, subscribe to news and information on the changes occurring in the system (for example, about the changes on the sites of any users), thematic forums and discussions, surveys and polls.

management process as the site as a whole and the entities within the site: page layouts, templates, O ‘

Design solutions in the development of intellectual repository of knowledge and automation of information support of managerial decision-making, together with the data mining technology, artificial intelligence methods, models, reporting, electronic databases on various subject areas will serve as a tool to improve the efficiency of research, innovative educational activities, as well as in industry, economics, medicine, and so on. d.

The practical implementation of the project allows you to use it as a self-adjusting, adaptive, open intellectual information system with integrated functions of expert systems! data mining (data mining).

Yablokov Denis
Senior Developer

The universal data model in theoretical materials science

SCIENTIFIC ORGANIZATION

Samara National Research University

ABSTRACT

The universal conceptual data model as a platform for creation of the databases containing information of any kind and any complexity is proposed. The methodology to describe chemical objects with different nature, properties and interrelations is developed. The terms framework containing a set of basic concepts and elementary primitives for classification and structuring of the described information is introduced. With this model, we have created a universal storage, which is used in our expert system for materials science.

KEYWORDS

Universal data model, expert system, materials science, object-oriented approach, relational database, elementary primitive, concepts refinement.

ACKNOWLEDGEMENTS

This work was supported by the Russian government (Grant 14.B25.31.0005).

SUMMARY

The problem of creation of universal data storage becomes significant in the case of implementation of unstructured data collection using an object-oriented approach for information representation and a relational database. The domain area is described by units of data, in accordance with some predefined concepts. The main concepts are: “meta-type”, “instance type”, “instance”, “hierarchy type” and “relationship attribute”. We define and describe additional concepts: “property descriptor”, “primitive property”, “composite property”, “category type”, “category”, “subcategory”, and “linked category”. These concepts determine a set of tables that fixes the entity-relation structure in the database. A unique feature of such approach is the possibility of arrangement of unlimited number of objects over a limited set of concepts. During research activity, it is important to process relevant and complete the information about the objects of different nature and properties. The universal data model allows storing information of any type and complexity by using elementary primitives to describe the hierarchical links and data relationships. As these primitives the data elements related to the basic concepts of graph theory, database theory, and programming are used. They allow one to construct the necessary abstraction level and to use different methodological approaches for data processing. For example, the conceptual framework in materials science is connected to definitions of graph theory that allows one to describe crystal-chemical data using graph abstractions. With interrelated concepts from chemistry and discrete mathematics we can classify the basic objects, such as atom or bond as well as more difficult objects, such as molecules, rings, ligands, nets, etc… Applying the concept of “is a” allows to store information on objects with similar behavior and to consider their relations as hierarchy by the principle “from the general to the particular”. Applying the concept “part of” allows storing information on objects and their relations, using the

principles of aggregation and composition. This allows considering their relationships in accordance with the principle “from the whole to the part”. The concept “is a” allows storing information about similar behavior of objects, such as atoms and void centers or bonds and channels. Concept “part of” allows describing the data hierarchies “atom–structure fragment–net” or “atom-bond-ring-tile”, etc. It is shown that the universal data storage is important part of expert system for materials science. It allows organizing the knowledge database to create and store strategic and meta-rules for more effective search of the decision in the process of predicting the properties for chemical substances of different classes.

Zarochentsev Andrey
Magister
Junior Researcher, engineer

Federated data storage system prototype for scientific applications

SCIENTIFIC ORGANIZATION

Kurchatov Institute

ABSTRACT

Rapid increase of data volume from the experiments running at the Large Hadron Collider (LHC) prompted national physics groups to evaluate new data handling and processing solutions. Russian grid sites and university clusters scattered over a large area aim at the task of uniting their resources for future productive work, at the same time giving an opportunity to support large physics collaborations.

KEYWORDS

BigData, Distributed storage, WLCG.

ACKNOWLEDGEMENTS

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SUMMARY

In our project we address the fundamental problem of designing a computing architecture to integrate distributed storage resources for LHC experiments and other data-intensive science applications and to provide access to data from heterogeneous computing facilities. Studies include development and implementation of federated data storage prototype for Worldwide LHC Computing Grid (WLCG) centers of different levels and university clusters within one national cloud.

The prototype is based on computing resources located in Moscow, Dubna, St.-Petersburg, Gatchina and Geneva. This project intends to implement a federated distributed storage for all kind of operations such as read/write/transfer and access via WAN from Grid centers, university clusters, supercomputers, academic and commercial clouds. The efficiency and performance of the system are demonstrated using synthetic and experiment-specific tests including real data processing and analysis workflows from ATLAS and ALICE experiments, as well running on supercomputer. We present topology and architecture of the designed system, report performance and statistics for different access patterns and show how federated data storage can be used efficiently by physicists and other scientists. We also describe how sharing data on a widely distributed storage system can lead to a new computing model and reformations of computing style, for instance how bioinformatics program running on supercomputer can read/write data from federated storage.

ADDITIONAL INFORMATION

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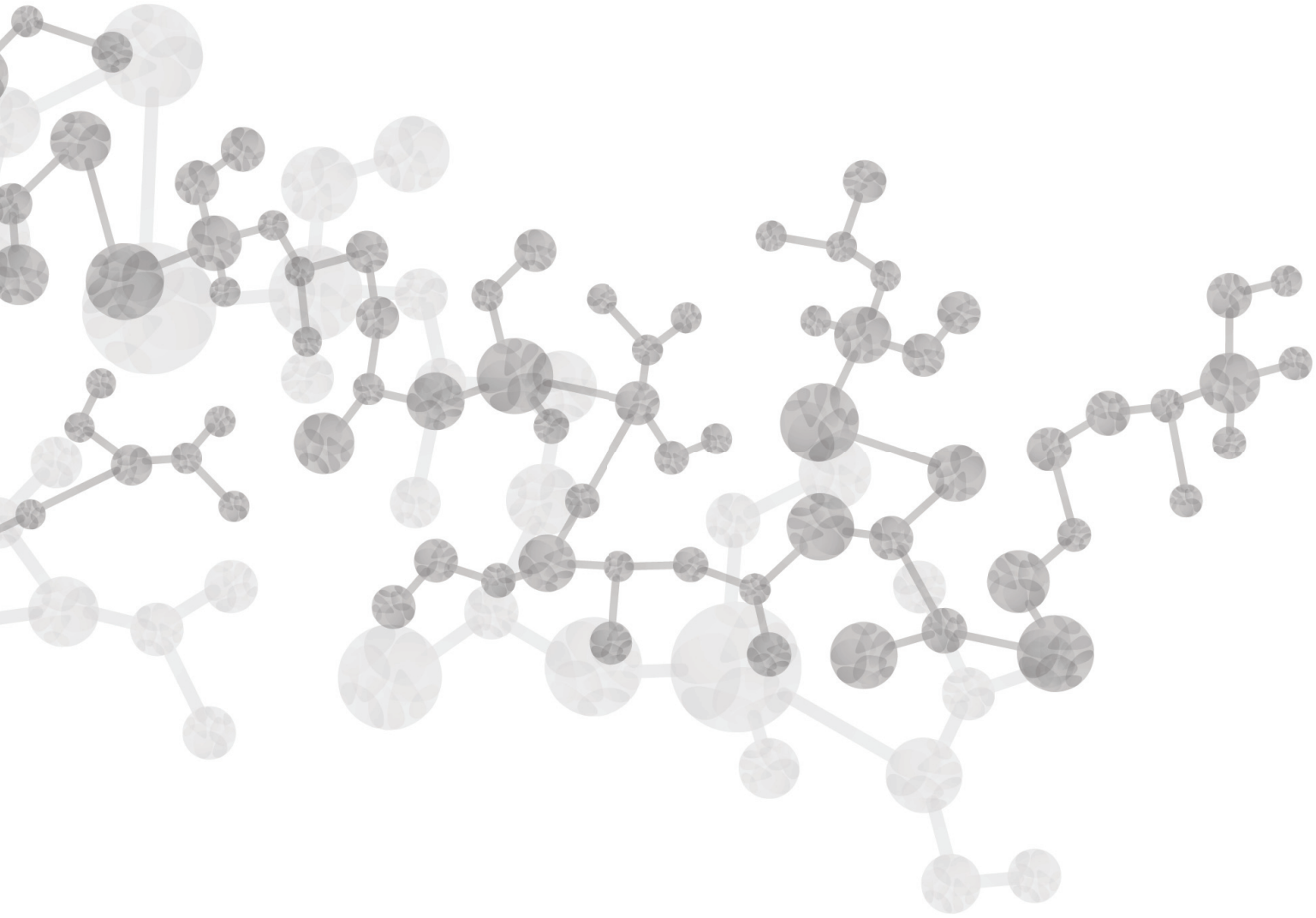

LIFE SCIENCES & MEDICINE

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Professor

Essential role of alpha-synuclein in brain energy metabolism – implication to health and neurodegeneration

SCIENTIFIC ORGANIZATION

University College London
Institute of Neurology

KEYWORDS

Alpha-synuclein, energy metabolism, mitochondria, brain.

ACKNOWLEDGEMENTS

This work was supported by Ministry of Education and Science of Russian Federation (Grant #14.616.21.0054) and BRC grant.

SUMMARY

Despite a strong implication of misfolded α-synuclein in Parkinson's disease, very little is known about the role of this protein in physiology. However, knowledge about a physiological role for unfolded, monomeric α-synuclein is limited. We have found an important function for alppha-synuclein in the regulation of ATP synthase activity. Applicatioon of extracellular monomeric α-synuclein enters the cell and localises to mitochondria, interacts with ATP synthase and modulates ATP synthase function. Using a combination of biochemical, live cell imaging and mitochondrial respiration analysis we found that lack of synuclein in mitochondria are uncoupled as characterised by increased mitochondrial respiration and reduced mitochondrial membrane potential. Furthermore, synuclein deficiency results in reduced ATP synthase efficiency and lower ATP levels. Exogenous application of monomeric α-synuclein is able to increase the ATP synthase activity that rescue the mitochondrial phenotypes observed in synuclein-deficiency. Overall, the data suggest that alpha-synuclein is a previously unrecognised physiological regulator of mitochondrial bioenergetics in brain cells through its ability to interact with ATP synthase and increase its efficiency.

ADDITIONAL INFORMATION

Co-autors: Alexey V. Berezhnov, Marthe H.R. Ludtmann.

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Tissue engineering models on the basis of human cardiac cells for the study of cardiac tachyarrhythmia

SCIENTIFIC ORGANIZATION

Moscow Institute of Physics and Technology

ABSTRACT

In the present study, we report on the development of tissue-engineering model that is based on human cardiomyocytes derived from cell reprogramming. It demonstrates the effectiveness of these models in assessing and determining the efficiency of antiarrhythmics cardiac pharmaceuticals. A patient-specific cardiac tissue models to explore mechanisms of deadly reentry - arrhythmias in patients with prolonged electrocardiographic QT interval is developed.

KEYWORDS

Tissue engineering, cardiomyocyte, cell reprogramming, excitation waves, cardiac arrhythmia, optical mapping.

SUMMARY

In recent years, tissue-engineering model based on the cardiac cells have shown to be effective in an experimental study of the mechanisms of cardiac arrhythmias, replacing the traditional electrophysiological preparations. These advantages include the good reproducibility and the ability to control tissue architecture via the

substrate topography or the architecture of the cultivation polymer matrices. Particularly functional, these models make use of a so-called optical mapping (using fluorescent dyes, marking excited heart cells) for visualization and registration of waves of excitation, controlling myocardial contraction.

With the aid of cultured cardiac tissue it was possible, for example, answer questions such as why certain patterns of conductive heart tissue are arrhythmogenic, how a so-called overdrive pacing can normalize cardiac rhythm, what is the mechanism of the drug suppression of a reentry source while decreasing the excitability of the myocardium, and others.

However, conventional tissue engineering myocardium models have a serious drawback due to the fact that they are based on animal (usually rat) cells. In this case, the set of ion currents through a rat cell membrane is significantly different from human. For example, in rats fast rectifying potassium current, Ikr practically is absent. This fact makes it unsuitable for a rat model any study of Class III antiarrhythmic drugs, which has been used successfully in medical practice and based on blocking Ikr. In the present study, we report on the development of tissue-engineering model that is based on human cardiomyocytes derived from cell reprogramming. The development of patient-specific cardiac tissue models to explore mechanisms of deadly reentry - arrhythmias in patients with the prolonged QT interval, recorded on the electrocardiogram, is also reported.

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SCIENTIFIC ORGANIZATION

Institute of Theoretical and Experimental Biophysics of RAS

Intercellular adhesion molecules of acute myeloid leukemia cells and drug resistance phenotype

ABSTRACT

We showed expression of CD11a, CD11c, CD18, CD54 on multicellular aggregates forming AML cells and expression of CD11a and CD18 only on multicellular aggregates not forming AML cells. Use of inhibitory antibodies to CD11a, CD18 and CD54 decreased formation of multicellular aggregates. We assume that in formation of multicellular aggregates and drug-resistance phenotype of AML cells may be involved intercellular adhesion molecule such as CD11a, CD18 and CD54.

KEYWORDS

Acute myeloid leukemia, drug resistance, intercellular adhesion.

ACKNOWLEDGEMENTS

The work was supported by the grant of Government of the Russian Federation №14.Z50.31.0028 and President of the Russian Federation Scholarship PS-1519.2015.4.

SUMMARY

One of the most important roles in the formation of drug resistance in acute myeloid leukemia (AML) cells plays adhesion to mesenchymal stromal cells and extracellular matrix of the bone marrow. Previously we have shown that the phenotype of drug resistance in AML cells may also occur when activated homotypic cell-cell adhesion in multicellular aggregates. In turn, the suppression of homotypic cell-cell adhesion prevents the formation of drug-resistance phenotype of AML cells. In this work, the identification of AML cell adhesion molecules was performed and the role of identified molecules in the activation of homotypic cell-cell adhesion was studied. In our study we used THP-1 cells (multicellular aggregates forming cells) and KG-1 cells (multicellular aggregates not forming cells). The identification of cell adhesion molecules was performed by flow cytometry with using monoclonal antibodies to human CD11a, CD11b, CD11c, CD18, CD50, CD54 and CD102. To study the role of the identified adhesion molecules in the multicellular aggregates formation AML cells were incubated with appropriate inhibitory antibodies. When intercellular adhesion was induced by PMA and number of newly formed

multicellular aggregates was counted. We showed expression of CD11a, CD11c, CD18, CD54 on THP-1 cells. In turn, on the KG-1cell expressed only CD11a and CD18. We also showed that the use of inhibitory antibodies to CD11a and CD18 decreased multicellular aggregate formation by THP-1 cells to 51 ± 6% relative to a control. Use of inhibitory antibodies to CD54 decreased formation of aggregates to 25 ± 4% relative to a control. In turn, the use of inhibitory antibodies to CD11c has no effect on formation of multicellular aggregate by THP-1 cells. Thus, in the formation of multicellular aggregates and drug-resistance phenotype of AML cells may be involved intercellular adhesion molecule CD11a, CD18 and CD54.

ADDITIONAL INFORMATION

Co-autors: Roman Fadeev, Irina Fadeeva, Anatoly Senotov.

Akhmetshina Dinara
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Junior Researcher

Nature of the early sensory input during the critical period of somatosensory system development

SCIENTIFIC ORGANIZATION

Kazan (Volga region) Federal University

ABSTRACT

The main finding of the present study is that endogenous (self-generated movements) and exogenous (stimulation by the littermates) mechanisms cooperate in driving activity of primary somatosensory cortex in the newborn rats and point on the importance of environment in shaping cortical activity during the neonatal period.

KEYWORDS

Neonatal rat, primary somatosensory cortex, critical period of the development, electroencephalogram, extracellular recording, whisker movements, tactile contact, natural environment.

ACKNOWLEDGEMENTS

The study was supported from the Russian Federation grant (11.G34.31.0075 to RK), the program of competitive growth of KFU, the subsidy allocated to KFU for the state assignment in the sphere of scientific activities and INSERM (LIA to RK).

SUMMARY

Sensory input plays critical roles in the development of the somatosensory cortex during the neonatal period. This early sensory input may involve stimulation arising from passive interactions with the mother and littermates but also sensory feedback arising from spontaneous infant movements. Relative contributions of these mechanisms under natural conditions remain largely unknown, however. Here, we used simultaneous high speed video recordings of whisker movements and extracellular multichannel silicone probe recordings of cortical barrel column activity. We show that in the whisker related barrel cortex of neonatal rats, spontaneous whisker and whisker pad movements and passive stimulation by the littermates cooperate, with comparable efficiency, in driving cortical activity. Both tactile signals arising from the littermate's movements under conditions simulating the littermate's position in the litter, and spontaneous whisker movements efficiently triggered bursts of activity in barrel cortex. Yet, whisker movements with touch were more efficient than free movements. Comparison of various experimental conditions mimicking the natural environment showed that tactile signals arising from the whisker movements with touch and stimulation by the littermates, support: (i) twice higher level of cortical activity than in the isolated animal, and (ii) three times higher level of activity than that supported by the deafferentated thalamocortical oscillator. Altogether, these results indicate that endogenous (self-generated movements) and exogenous (stimulation by the littermates) mechanisms cooperate in driving cortical activity in the newborn rats and point on the importance of environment in shaping cortical activity during the neonatal period.

Alkon Natalia
Master
Student

Searching for Vicugna pacos VHHs against cancer stem cell markers CD44 and ERBB2 with the help of ribosome display

SCIENTIFIC ORGANIZATION

M.M. Shemyakin and Yu.A. Ovchinnikov Institute of bioorganic chemistry of the Russian Academy of Sciences

ABSTRACT

Vicugna pacos single-chain antibodies (VHHs) against cancer stem cell (CSC) markers might provide a valuable tool for cancer immunotherapy, which is considered as a substantial supplementation to traditional ways of treatment. Ribosome display helps with finding specific VHHs against such well-known CSC markers as CD44 and ERBB2.

KEYWORDS

Immunotherapy, single-chain antibodies, VHH, ribosome display.

ACKNOWLEDGEMENTS

The results of this project were achieved with support of the Ministry of Education and Science of the Russian Federation as a part of the agreement 14.607.21.0062 of the Federal Special-Purpose Program “Research and development in the high priority development fields scientific and technological complex of Russia for 2014-2020”.

SUMMARY

Today one of the most promising ways of cancer treatment is immunotherapy. *In vitro* experiments showed that co-cultivation of cancer cell line RKO with lymphocytes, activated by dendritic cells, which were maturated in presence of the RKO cancer cell protein lysates, lead to significant 98% RKO cells growth inhibition. However, *in vivo* experiments require methods with better specificity, such as chimeric antigen receptors (CARs) carrying selective antibody structures. CARs endue effector immune cells with significantly elevated specificity towards their molecular targets. Probably one of the most convenient ways of designing such CARs is based on *Camelidae* single-chain antibodies. Not only are they shorter than usual antibodies – about 500 bp – which ensures a wider range of applications, but also sometimes such antibodies demonstrate higher selectivity to their molecular targets. Ribosome display is a simple and straightforward method for rapid evolution and selection of protein ligands, and in particular, for selection of antibodies. With this technology selecting from libraries with high complexity (about 10^15) becomes possible. This in turn allows analyzing naive libraries, the diversity of which is higher, as well as reduces time and efforts. Specific heavy-chain variable domain (VHH) of *Vicugna pacos* antibody against CD47 – one of the well-known cancer stem cells (CSCs) markers – was previously found with phage display technology. The upstream region for cell-free coupled transcription-translation and downstream sequence containing either Flag-tag alone, or in conjunction with tRFP-tag, followed by the constant region of immunoglobulin kappa light chain (Ck) with removed stop codon were added to the aforementioned anti-CD47 VHH sequence with OE-PCR. Ribosome display selection cycle based on this construct turned out to be fully functional, as mRNA-ribosome-VHH complexes required for ribosome display were produced. Afterwards, VHH libraries were prepared: naive library from the lymph node of neonate alpaca, and immune library from ERBB2-immunised animals. Several selection cycles were carried out with ribosome display technology using constructs, which were obtained on the bases of such naive and immune libraries in order to find selective antibodies against cancer stem cell markers CD44 and ERBB2 correspondingly.

Andreeva Tatiana
PhD
Senior Researcher

The whole mitochondrial genome sequences from specimens of ancient Siberian Tagar and Pazyryk cultures vanished in the first century BC: implications to their origin and medical history

SCIENTIFIC ORGANIZATION

The Federal Research Center Institute of Cytology and Genetics of Siberian Branch of the Russian Academy of Sciences

ACKNOWLEDGEMENTS

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SUMMARY

The genetic replacement of the Mesolithic populations during the Neolithic in Europe and Asia is not yet well elucidated. The Tagar (upper reaches of Yenisei river) and Pazyryk (Altai) cultures both flourished during the Scythian period of Siberia history (first millennium BC) and became exceptional in livestock breeding, metal production and arts. Both bronze and iron casting have been mastered for production of tools and weapons. As others in southern Siberia, they had a highly developed artistic culture of Scythian-Siberian animalistic style. Interestingly, trepanning is one of the oldest surgical procedures which has archaeological evidence, and, among other places, ancient trepanned sculls have been discovered in Pazyryk culture sites.

We extracted DNA from two ancient tooth specimens (one of Tagar culture individual and one of Pazyryk culture subject with trepanned scull) and prepared deep sequencing libraries using modified single-stranded DNA protocol to increase the highly degraded DNA yield and to exclude contamination with modern samples. Using deep sequencing with Illumina HiSeq 2500, we generated short read sequencing data and reconstructed whole mitochondrial genome sequences for Pazyryk and Tagar samples. The authenticity of DNA was confirmed by the observed specific ancient DNA signatures: short DNA fragments and elevated rates of C->T substitutions towards fragment ends. The potential contamination of modern DNA was estimated by Schmutzi program testing of 256 Eurasian population haplotypes. After excluding potential minor contamination with modern DNA (1-3%), we reconstructed almost complete mitochondrial genome sequences and identified haplogroups for both samples.

We found haplogroup F1b1b for the Tagar subject and U5b2b for the Pazyryk subject. These haplotypes are presented in both Asian and European populations. The F1b is relatively frequent as a fraction of total F in northern parts of East Asia and Central Asia and frequent in Tai peoples. The U5b has been found in remains dating from prehistoric times in Europe. Therefore, the common view is that ancient European mitochondrial haplogroup, U5, arose in Europe. The coalescence time is ~20–24 ky (thousand years) for U5b haplotype. The frequency of U5 haplotypes in Neolithic and present day populations (1-8 %), is lower than in Mesolithic (except Saami populations). Previously, unexpectedly widespread presence of U5b was noted for ancient Mesolitic samples across Europe. We showed the finding of this haplotype in ancient Siberian culture with elements of early advanced medical history. The data show surprisingly uniform presence of U5b in ancient human populations extended from Europe to Asian Siberia. The data suggest the origin of widespread ancient human populations from small number of founders with U5 haplotype expanded to vast historical time-span and geographic areas.

ADDITIONAL INFORMATION

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Emotion regulation features of foster Infants

SCIENTIFIC ORGANIZATION

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ABSTRACT

Emotional regulation (ER) considered in the context of infant attachment. Children living in different conditions of family environment may have quantitative and qualitative differences in the styles of ER (constructive, destructive). We consider three groups of children: traditional-type of baby home, family-type of baby home and foster families. DAM evaluates the emotion expression of the child and caring adult in 5 situations. Stressful situations (separation from adults) should activate most frequently used ER strategies that will enable us to assess their effectiveness.

KEYWORDS

Foster care, institutionalization, Baby Home, emotion regulation, DAM.

SUMMARY

Introduction

In the middle of last century Early Intervention Psychology has identified the importance of social and emotional development of man in early childhood and its impact on the rest of his life. Particular attention was paid to the emotional relationship between child and mother in connection with the separation from her in the period of hospitalization (Bowlby, 1969; Ainsworth, 1978). Concerning to date there is no doubt that the sensitive period for the construction of an emotionally stable relationship between mother and child is the early childhood (Mahler, 1975; Winnicott, 1949, 1965; Stern, 1985; Klein, 1920). It is also known that the presence of constant close adult in the absence of the mother may somehow offset the effects of deprivation (Elinor W. Ames, 1997).

The most striking example of such a study is a project with Romanian orphanages, when some of them were adopted by families from Canada. Early-adopted group of Infants (before they were 4 month of age) were for the most characteristics of social-emotional development as a Canadian-born group (never-institutionalized children living with their birth parents), but there were many differences between this 2 groups and Romanian children, who had spent somewhere between 8 and 53 month in orphanage.

Children abilities to understand and accept their own emotions largely depend on feedback from mother/close adult. The lemmas of emotional control strategies in future is resolving specific to early childhood (2-3 years) of the internal contradictions. Such conflicts may arise because of strong experiences during the frustrating situation, which are caused by short or long-term separation from care adult (mother). Mother's sensitivity to children emotion conditions determined how an Infant would regulate own affects. The influence of the social environment (mostly family) on the emotional sphere of the child is described in detail in many foreign issues (Morris, Silk, Steinberg, Robinson, 2007; Ramsden, & Hubbard, 2002; et al.). Therefore we are interested in the situation of institutionalized children and foster families, because there are many studies of institutionalized effects to child mental health and physiology. For example, institutionalization were considering like early-life stress, such as maltreatment and exposure to violence, which associated telomere shortening (Asok, Bernard, Roth, Rosen, Dozier, 2013). Authors found association between early-life stress (high-risk children) and telomere length; also they examined the role of parental responsiveness in buffering children from telomere shortening following experiences of early-life stress. Next groups of studies are connected with cortisol (stress hormone) production. It was examined differences in level of cortisol between children from biological (birth parents) and foster families. High-risk children who were living with birth parents had more high level of cortisol in waking to bedtime then children placed in foster care (Bernard; Butzin-Dozier; Rittenhouse; Dozier). We can observe how environments influence to children. Another interesting result is connected with attachment and cortisol level. Infants with attachment disorganization showed cortisol's increasing in Strange Situation then organized infants (Bernard, Dozier, 2010). In orphanage more children have disorganization type of attachment (not secure attachment) that's why in

stress (strange) situation they don't use constructive strategies of emotion regulation (Muhamedrahimov, 2009).

Also we wanted to notice studies with Infant's emotional regulation. In study where researches assess emotional expression in child's face, they found some phenomena connected with negative and positive affects: children in orphanage show less negative affects in separation-reunion (stress) situation with care adult and more positive affects. Why happened this? Why we see increasing positive affects when infant should demonstrate sadness or angry (adult leave him in play time without warning)? Authors explain that fact as a specific characteristic of strategy to achieve the goal. Objective might be an attention of care adult, strategy to keep connection and regulate own emotions (Muhamedrahimov, 2008). This is an example of how the children do not learn to express their negative affects in a constructive manner, thereby hidden negative emotions found other ways to exit (eg, stereotypes and aggression).

Emotional sphere and ways of its regulation are inextricably linked with cognitive and behavioral processes of the child's psyche. It is also stable and balanced emotional state is a prerequisite for the development of intellectual processes. Thus, a child who is constantly experiencing severe emotional distress and can't regulate them (constructive ways) will be different from the one who has developed (from care adult) emotional regulation strategies, enabling it to function properly.

Describing these studies we want to demonstrate the importance and urgency of the problem being studied. In this study we are interested in the possibility of compensating the family of the consequences of deprivation in children. With the development of the adoption system and practice of placing children in foster families increases the relevance of studying the characteristics of the most dominant areas in child's regulation at this age period - emotional. Due to the fact that children have not yet formed a system of self-regulation and emotion exhibited by them are more biological rather than social, i.e. more sincere and truthful, so it is possible to observe their expression through verbal and non-verbal components in situations of interaction with care adults, as well as the situation in his absence (stressful, frustrating situation). It is also known that the foundations of emotional regulation are laid in early childhood (Eisenberg, Spinrad, Eggum, 2010). So what strategies can be used by children to regulate their condition (emotions, behavior)? According to the observations of children in the experiment with marshmallow authors identified frequently used effective strategies (Eisenberg and Sulik, 2012):

1. Shifting attention away from a distressing stimulus or a tempting object can decrease arousal;

2. Focusing attention on positive aspects of the situation or on other means of coping also can decrease negative emotion;

3. Verbal control in the form of speech or singing;

4. Focus on the desired subject (less efficient).

This is only a small part of the repertoire of emotional regulation infants. Each situation is forcing to use one or the other (better acceptable) style of regulation. In a broader sense, even crying and screaming child a means of emotional regulation. But what kind of strategy will be presented in the repertoire of the child depends on many aspects: temperament, family background, marital relations and conflicts (Cummings, Davies, 2002), physical and mental health (Stansbury, Gunnar, 1994), gender (Chaplin, Cole, Zahn-Waxler, 2005), quality of relationships with adults and peers (Contreras, Kerns, Weimer, Gentzler, Tomich, 2000), etc.

It is not enough studied foster care system due to the emotional development of the child as an independent person and in the context of building an emotionally stable relationship with a close adult.

The above problems are not characteristic of all institutionalized children. Children from family-type baby homes may differ significantly from children in traditional-type baby homes. Also the differences may be related to culture, place, social environment characteristics. Children from China and Eastern Europe (institutionalized) participated in two tasks on the understanding of emotions: it was necessary to choose the image with the appropriate facial expressions of emotion (joy, sadness, anger and fear) and then identify facial expressions in history, describing the characteristic of these emotions situations.

While the group of institutionalized children got lower results compared with the control group (never- institutionalized), children from China show better results in

emotion understanding than children from Eastern Europe. Post-institutionalized children's performance was predicted by their age at adoption (Camras, Perlman, Fries, Pollak, 2006).

We mentioned a little about the causes that underlie the effects of deprivation - a dysfunctional relationship of the child and care adult, disorganization attachment. With regard to children from baby homes there is a lot depends on the pace of life and daily routine in which the children reside. Caregiver should observe to the whole group (6 to 15 children) did not allow him to pay due attention to each child. To build a secure attachment, strong relationships that will act as a resource for the child require special organization of the environment (in the broad sense).

In the study examined time use of children in Russian baby homes are presented detailed results of how much time and what to spent the children: 50% of the time they spent alone, 27% with a caregiver, 15% with another adult and only 7% with other children. The younger the child, the more time a child spends alone (infants to 65%). Children spend a lot of time on non-purposeful activity (Tirella, Chan, Cermak, Litvinova; Salasand, Miller, 2007).

Measures with videotaping became very popular in assess attachment, emotions, behavior etc. They have proven their validity and reliability (Clark, 1999; Muhamedrahimov, 1999).

Methods

Participants

For the pilot study participants included 30 couples (infant-care adult) of ranging in age from 8 to 48 month:

- Foster families – 10 couples
- Traditional-type of Baby Home – 10 couples
- Family-type of Baby Home – 10 couples

Measures

DAM (Dyadic Affect Manual, Osofsky, Muhamedrahimov, Hummer, 1998).

We used the DAM to assess quantitative and qualitative characteristics of emotion expression and Infant's behavior in interaction and separation situations. To study the emotion we produced video of Infants and their care adults in five situations, namely:

1 – free play (3 minutes)

2 – first separation (care adult leave a room for 3 minutes)

3 – first reunion (care adult comes back in to the room and play with child for 3 minutes)

4 – second separation (care adult again leave a room for 3 minutes)

5 – second reunion (care adult comes back in to the room and last time play with child for 3 min).

Instruction for parents: "Play please with child the way you usually do. When you hear a signal as knocking please leave the room and come back with next knocking. You have to leave the room twice, but the second time you should warn the child like 'I'm going out', 'I will come back' etc. By the way you can return at any time if you want".

The diagnostic purpose of separation and reunion episodes is to assess the child's response to a situation of frustration and the change of emotional state when care adult returns.

In a situation of frustration remaining alone children express / suppress their emotions or use some emotion more often, then others and can vary the intensity. All this can be considered as an emotional regulation strategies.

In each episode, three minute intervals allocated for 30 seconds and coded next indicators:

- 4 positive affects (joy, interest, excitement, surprise)
- 4 negative affects (distress, sadness, anger, fear)
- Gross motor

- Manipulative
- Stereotype movements
- Aggression to object
- Aggression to people

The intensity of each emotion is estimated from 1 to 5 points and then coder chooses the maximum intensity of each emotion for the episode. In addition calculated the sum of all positive (general positive emotional tone) and negative affects (general negative emotional tone).

Object: emotional regulation

Subject: emotions and behavior characteristics of Infants in foster families

The **hypothesis** of the study: we expect that infants in 3 groups will have different characteristics of emotion regulation because of their social environment. Namely, children in foster care group will use less dysfunctional forms of emotional regulation than children from 2 Baby Homes.

Results

This study is conducted on the basis of the grant “Influence of early deprivation on biological and behavioral indicators of child development”, supported by the Government of the Russian Federation. The results, which we will get to September in to pilot study will help us to understand in which direction should move on. And on this basis we hope to formulate recommendations for the employees of baby homes, the foster parents, professionals (psychologists, psychotherapists, and others.). All data (a video) are analyzed by specially trained people with appropriate qualifications and the level of consistency in the results of at least 95%.

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Use of Semiconductor Nanocrystals to Encode Microbeads for Multiplexed Analysis of Biological Samples

SCIENTIFIC ORGANIZATION

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)

ABSTRACT

Microbeads encoded with semiconductor quantum dots (QDs) are suitable tools for multiplexed analyses of various biological markers using flow cytometry. We used layer-by-layer deposition to obtain populations of microbeads encoded with QDs with different colors and intensities of fluorescence. This method allows QDs to be separated with one or several polymer layers in order to prevent Förster resonance energy transfer (FRET) and the resultant quenching of QD fluorescence in multicolor microbeads.

KEYWORDS

Nanocrystals, Förster resonance energy transfer, microbeads, fluorescence.

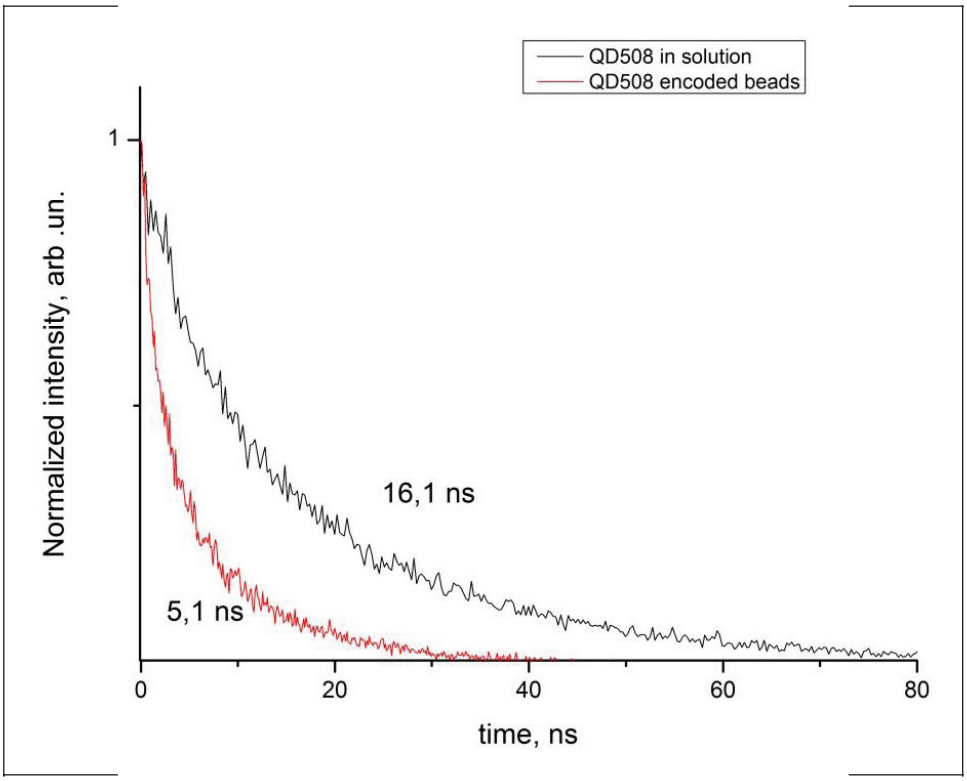
ACKNOWLEDGEMENTS

This study was supported by the Federal Targeted Program for Research and Development of the Ministry of Education and Science of the Russian Federation (grant no. 14.578.21.0054, contract no. RFMEFI57814X0054).

SUMMARY

In recent years, interest in optically encoded microbeads has been growing due to their potential applications in medical diagnostics [1]. Microbeads can be encoded with either organic fluorophores or semiconductor quantum dots (QDs) [2-6]. Quantum dots constitute a new class of fluorophores that have a number of advantages over routinely used fluorescent organic dyes, such as a high brightness, resistance to photobleaching, a wide excitation spectrum, and a narrow emission one [8-9]. The unique optical characteristics of QDs make it possible to use them in multiplexed analyses, as well as in multicolor imaging [10], because QDs of different colors can

Figure 1. Fluorescence lifetime of QDs 508 nm in a solution and adsorbed on microbeads



be simultaneously excited using a single radiation source, whereas their fluorescence peaks can be effectively separated and detected in different channels of a flow cytometer. Therefore, multiplexed analysis by means of flow cytometry using QD-encoded microbeads is easy to perform and does not require sophisticated equipment.

To obtain a population of microbeads encoded with QDs with different fluorescence peaks and fluorescence intensities, we used the method of layer-by-layer deposition [7]: the surface of microbeads was successively coated with layers of differently charged polyelectrolytes and negatively charged QDs. The number of QDs adsorbed on each microbead 4.08 μm in diameter was $1.8–2 \cdot 10^6$. The fluorescence lifetime and the degree of fluorescence quenching were measured to analyze Förster resonance energy transfer (FRET) for QDs in the solution and QDs adsorbed on the encoded microbeads. The fluorescence of the adsorbed QDs was quenched more strongly than that of suspended QDs. However, we cannot conclude that FRET occurred between the absorbed QDs, because the QD fluorescence lifetime was the same for microbeads encoded with one and several layers of QDs.

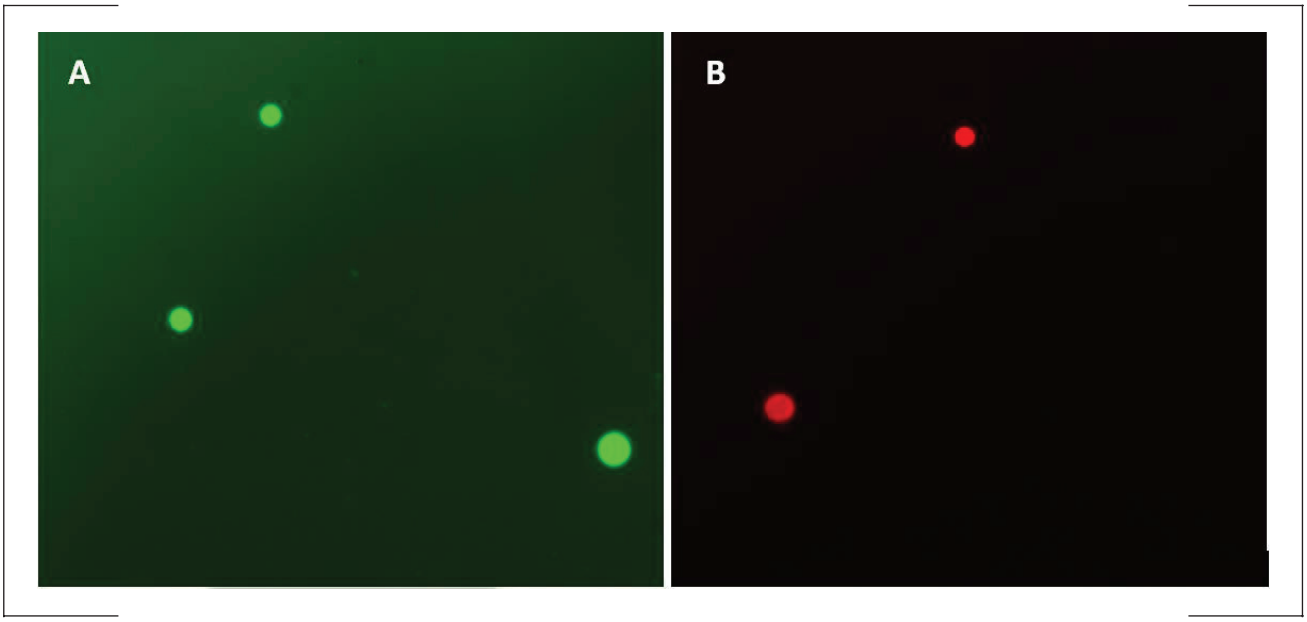


Figure. 2. Typical fluorescence microscopy images of microbeads of different sizes encoded with QDs 508 nm (A) or QDs 590 nm (B)

Populations of QD-encoded microbeads have been studied in detail using immunofluorescence. The technique of optical encoding of microbeads with QDs developed in this study makes it possible to obtain microbead populations for multiplexed analysis of biological markers using flow cytometry.

ADDITIONAL INFORMATION

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ABSTRACT

Store-operated calcium channel complex in postsynaptic spines: a new therapeutic target for Alzheimer's disease treatment. Elena Popugaeva1, Ekaterina Pchitskaya1, Hua Zhang2, Suya Sun2, and Ilya Bezprozvanny1,2 1Laboratory of Molecular Neurodegeneration (LMN), St Petersburg State Polytechnical University, St Petersburg, 19525, Russia 2Department of Physiology, University of Texas Southwestern Medical Center, Dallas, TX 75390, USA.

KEYWORDS

Alzheimer's disease, synapse, calcium signaling, imaging, neurodegeneration.

ACKNOWLEDGEMENTS

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SUMMARY

Mushroom dendritic spine structures are essential for memory storage. In the previous studies we suggested that the loss of mushroom spines may explain memory defects in aging and Alzheimer's disease (AD). We further demonstrated that the stability of mushroom spines depends on STIM2-mediated neuronal store operated calcium (Ca^{2+}) influx (nSOC) pathway which is compromised in AD mouse models, in aging neurons and in sporadic AD patients (Sun at al, 2014, Neuron, vol 82, pp 79-93; Zhang at al, J. Neuroscience, vol 35, pp 13275-13286; Popugaeva at al, 2015, *Molecular Neurodegeneration*, 10:37). The molecular identity of channel encoding SOC influx in spines remains unknown. We now demonstrate that TRPC6 and Orai2 channels form a STIM2-regulated nSOC Ca^{2+} channel complex in hippocampal mushroom spines. We further demonstrate that a known TRPC6 activator hyperforin and a novel nSOC positive modulator NSN21778 can stimulate activity of nSOC pathway in the spines and rescue mushroom spine loss in both presenilin and APP knock-in mouse models of AD. We further show that NSN21778 rescues hippocampal long-term potentiation impairment in APP knock-in mouse model. We conclude that STIM2-regulated TRPC6/Orai2 nSOC channel complex in dendritic mushroom spines is a new therapeutic target for treatment of memory loss in aging and AD and that NSN21778 is a potential candidate molecule for therapeutic intervention in brain aging and AD.Mushroom dendritic spine structures are essential for memory storage. In the previous studies we suggested that the loss of mushroom spines may explain memory defects in aging and Alzheimer's disease (AD). We further demonstrated that the stability of mushroom spines depends on STIM2-mediated neuronal store operated calcium (Ca^{2+}) influx (nSOC) pathway which is compromised in AD mouse models, in aging neurons and in sporadic AD patients (Sun at al, 2014, Neuron, vol 82, pp 79-93; Zhang at al, J. Neuroscience, vol 35, pp 13275-13286; Popugaeva at al, 2015, *Molecular Neurodegeneration*, 10:37). The molecular identity of channel encoding SOC influx in spines remains unknown. We now demonstrate that TRPC6 and Orai2 channels form a STIM2-regulated nSOC Ca^{2+} channel complex in hippocampal mushroom spines. We further demonstrate that a known TRPC6 activator hyperforin and a novel nSOC positive modulator NSN21778 can stimulate activity of nSOC pathway in the spines and rescue mushroom spine loss in both presenilin and APP knock-in mouse models of AD. We further show that NSN21778 rescues hippocampal long-term potentiation impairment in APP knock-in mouse model. We conclude that STIM2-regulated TRPC6/Orai2 nSOC channel complex in dendritic mushroom spines is a new therapeutic target for treatment of memory loss in aging and AD and that NSN21778 is a potential candidate molecule for therapeutic intervention in brain aging and AD.

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Dynamic of prefrontal-cortex transcriptome profiles in mice exposed to social defeat stress

SCIENTIFIC ORGANIZATION

Inctitute Cytilogy and Genetics SD RAS

KEYWORDS

Social defeat stress, depression, RNA-seq, prefrontal cortex.

ACKNOWLEDGEMENTS

This work has been done by the finance support of the Government of the Russian Federation (Project №14.B25.31.0033, Resolution No.220 Federation of April 9, 2010).

SUMMARY

Chronic social defeat stress is a well-validated murine model of depression. We aimed to study dynamic changes of genes expression during development of depression-like state in C57BL/6 mice. We analyzed the effects of social defeat stress of varying duration (10 and 30 days) on the behavioral patterns and prefrontal-cortex transcriptome in C57BL/6 mice. Commonly used 10-day exposure to defeat stress resulted only in a high level of social avoidance. Contrariwise, most mice exposed to 30-day stress demonstrated clear hallmarks of depression, including higher level of social avoidance, increased immobility in the forced swim test, and anhedonic behavior. Surprisingly, an analysis of RNA-seq data revealed massive changes on the 10th day, but a few ones on the 30th day of stress due to a reversal of most of the stress-induced changes to the initial state. We have found that glucocorticoid target genes stop responding to the elevated corticosterone level after 30-day stress. The majority of genes altered by 30-day stress were down-regulated, with the most relevant ones being *Robo3* participating in neurodevelopment and cell adhesion and some other cell adhesion molecules.Taken together, our data suggest that depression may be caused by weakening of the response to the stressful environmental factors in terms of both behavior and gene expression. Our results also support the hypothesis that major depressive disorder is associated with defective cell adhesion and impaired neuronal plasticity.

This work has been done by the finance support of the Government of the Russian Federation (Project №14.B25.31.0033, Resolution No.220 Federation of April 9, 2010).

ADDITIONAL INFORMATION

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Semiconductor quantum dot toxicity in a mouse in vivo model

SCIENTIFIC ORGANIZATION

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ABSTRACT

Quantum dots (QDs) are increasingly more used in clinical medicine. Their most promising potential applications are cancer diagnosis, including in vivo tumour imaging and targeted drug delivery. In this connection, the main questions are whether or not QDs are toxic for humans and, if yes, what concentration is relatively harmless. Here, we carried out in vivo experiments with the fluorescent semiconductor CdSe/ZnS core/shell QDs, which are currently the most widely used in research.

KEYWORDS

Quantum dots, toxicology, cancer in vivo imaging.

ACKNOWLEDGEMENTS

To the Federal Target Program for Research and Development of the Ministry of Education and Science of the Russian Federation (grant no. 14.584.21.0012, contract no. RFMEFI58415X0012)

SUMMARY

Quantum dots (QDs) are highly fluorescent inorganic semiconductor crystals with a diameter from 2 to10 nm (1). They can consist of a semiconductor core (CdSe, CdS, CdTe, InP, InAs, or PbSe) alone, or have a core/shell structure (usually, with a ZnS shell), the shell protecting the QD from oxygenation and enhancing the photoluminescence quantum yield (2). Regarding optical properties, semiconductor QDs are characterized by an exceptionally bright photoluminescence and rock-solid photo- and chemostability. They have broad quasi-continuous absorption and narrow, sharp emission spectra with an approximately Gaussian shape and large (>100 nm) Stocks shifts (3). The high brightness of fluorescent QDs is a result of high molar adsorption coefficients (several times higher than those of fluorescent dyes and proteins) combined with a high quantum yield (4). Moreover, different populations of QDs can be excited at the same wavelength, which can be very far from their respective emission bands, depending on the QD core size and composition. The size of QDs can be varied in the process of their synthesis, and the QD fluorescence color depends directly on their diameters.

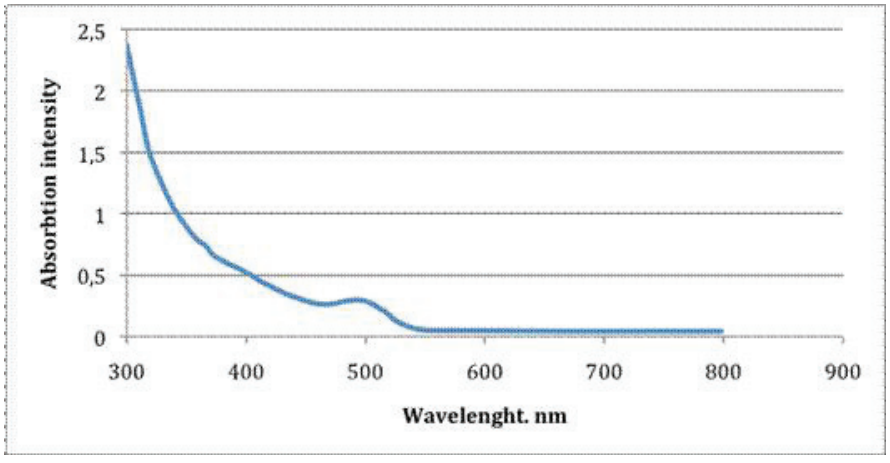
In recent years, QDs have been increasingly widely used in biology for cell targeting, imaging, and drug delivery due to their unique optical and physicochemical properties (5). They are likely to replace the commonly used organic dyes because of their considerable advantages over the organic fluorophores (6).

In addition, QDs are increasingly used in clinical medicine. Their most promising potential applications are in cancer diagnosis, including in vivo tumor imaging.

Cancer remains one of the leading causes of death in the world (7). One of unsolved problems is differentiation of tumor-affected tissue from healthy tissue during surgery. In addition, noninvasive determination of metastases is highly demanded. These problems can be solved by using *in vivo* tumor imaging. Many researchers address the issue of selecting the best method for *in vivo* tumor imaging using different substances, such as fluorescent proteins (8–13). Advanced optical characteristics compared to organic dyes determine the necessity of investigation of different aspects of QD use for *in vivo* optical imaging of tumors. In this connection, the behavior of QDs in living organisms is of special interest. Certainly, the main questions are whether or not QDs are toxic for humans and, if yes, what concentration of QDs is relatively harmless.

We have carried out *in vivo* experiments with fluorescent semiconductor CdSe/ZnS core/shell QDs, which are currently the most widely used in research. QDs coated with trioctylphosphine oxide (TOPO) were synthesized, solubilized, and modified with electrically neutral derivatives of polyethylene glycol (PEG) containing both thiol and carboxyl groups to make them soluble in water and aqueous buffer solutions and protect them from clustering (14).

Figure 1. The absorption spectrum of CdSe/ZnS core/shell quantum dots



Several stages of purification after coating QDs with PEG were performed so as QDs not to bear any toxic admixtures, such as unbound PEG or other substances. The stability of QDs was accurately measured during one month before the experiments in three different solutions, phosphate buffer, RPMI medium, and mouse blood serum, at different temperatures: room temperature and animal body temperature (37°C). Since QDs were stable under all these conditions, we could be sure that they would not aggregate or decompose

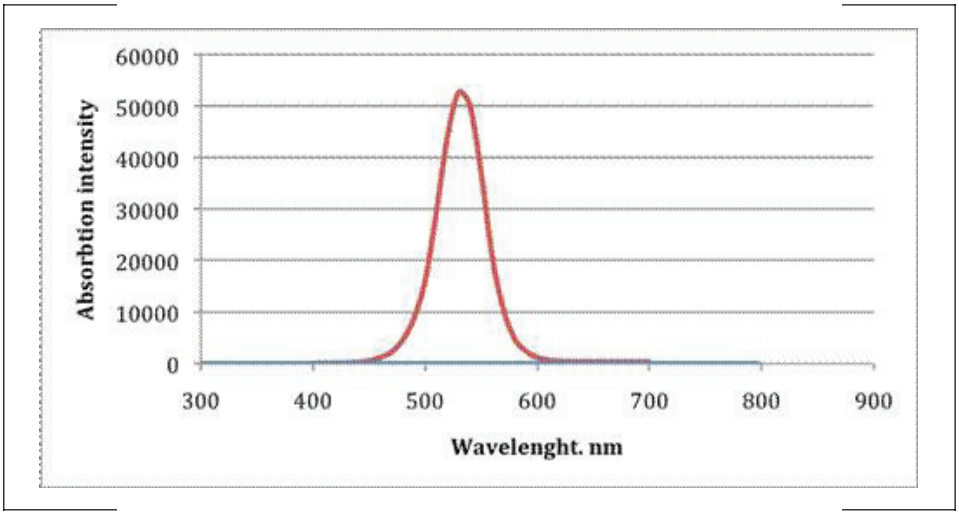


Figure 2. The emission spectrum of CdSe/ZnS core/shell quantum dots

shortly after they enter a living body. In addition, the physical characteristics of QDs, including their sizes and emission and absorption spectra (Figures 1, 2), were measured before *in vivo* experiment.

70 DMA/B6 hybrid mice were used to estimate the QD toxicity *in vivo*. A QD solution was injected intravenously. Pure solvent and PEG solution were used as negative controls. The mice were examined for about one month after QD injection. The survival rate was estimated throughout the study. Only in the group with the highest concentration of QDs did animals start to die during this period (survival rate, 75%).

During the experiment, we visually accessed the state of health of every animal and measured its weight (Figure 3). No significant weight loss was observed during four weeks.

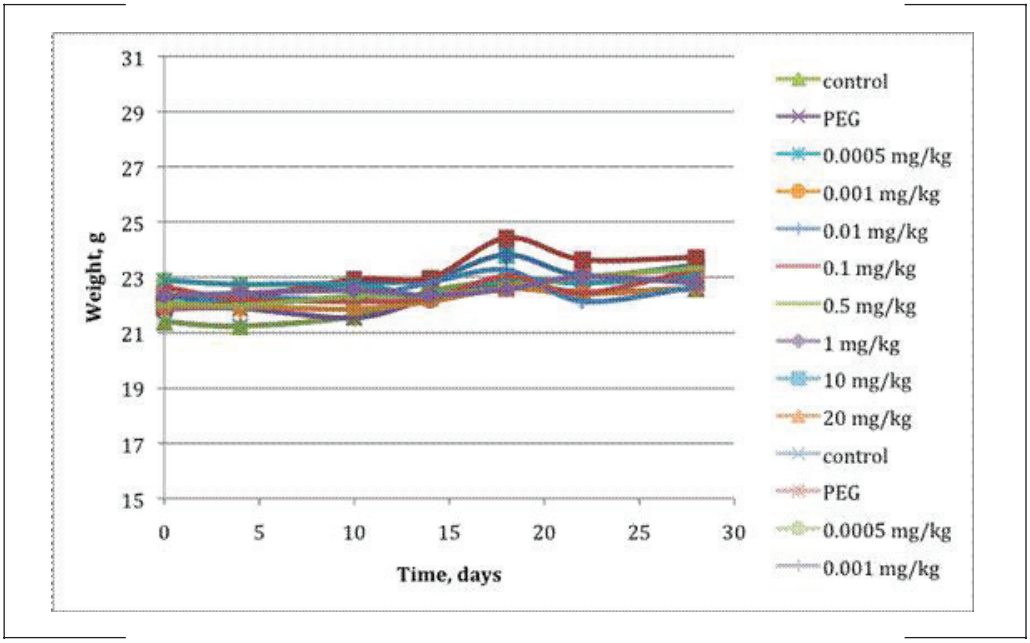


Figure 3. Animal weight assessment during the experiment

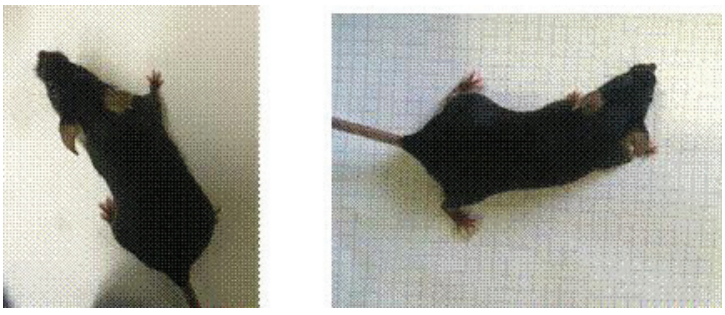


Figure 4. A mouse before the experiment (left) and a mouse three weeks after the injection of 10 mg/kg of QDs (right)

Special attention was paid to the state of the animals' hair and eyes. It was found that mice tolerated QDs well even at a concentration as high as 10 mg/kg. The mouse hair, teeth, and eyes looked like those of healthy animals (Figure 4).

One month after the injection, the internal organs were investigated. We used paraffin sectioning and haematoxylin–eosin staining to assess the state of the liver and kidney every week during four weeks. Their morphology was the same as in healthy control mice (Figure 5).

These results allow us to conclude that CdSe/ZnS QDs have no considerable toxic effect in the mouse in vivo model at concentrations up to 10 mg/kg, because there were no changes in organ morphology, physical parameters, and visually assessed general condition of mice and no weight variation during the four weeks of the experiment.

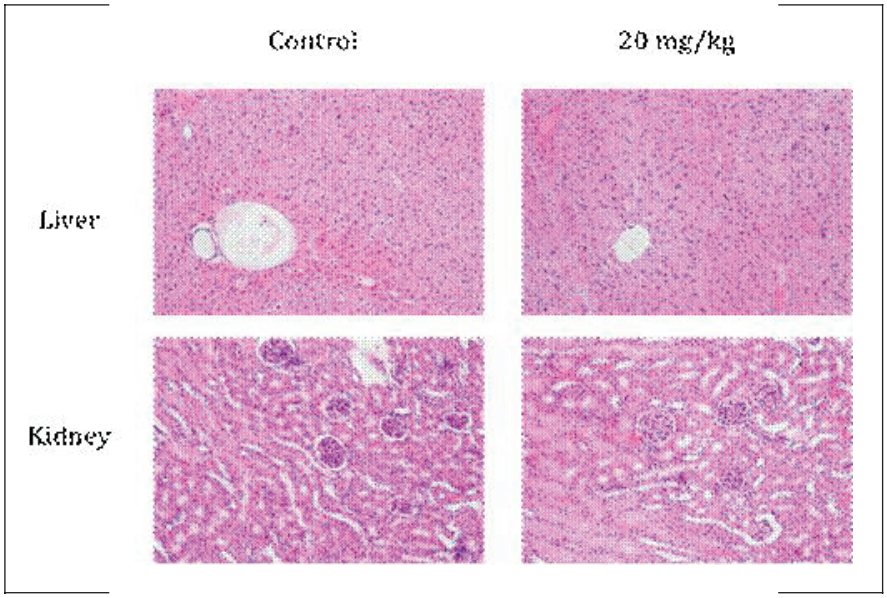


Figure 5. Liver and kidney haematoxylin–eosin staining at the fourth week of the experiment

However, the QDs were found to be toxic at the highest concentration studied, 20 mg/kg body weight, whith two-thirds of the animals dying shortly after the experiment was started. Further investigations will be performed to compare the single doses used in this experiment and the minimum therapeutic dose for these mice, so that we be able to use this mouse model for testing clinical applications of QDs.

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ADDITIONAL INFORMATION

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Тенденции и проблемы современной биотехнологии

SCIENTIFIC ORGANIZATION

INSERM U1106, Aix-Marseille University, Institute of System Neurosciences

SUMMARY

На протяжении тысячелетий человечество использовало биотехнологии в растениеводстве, производстве продуктов питания и в медицине. Современная биотехнология включает применение методов генной инженерии и модификации генетического материала для улучшения функций клеток или производства новых биологически важных компонент. Новые направления биотехнологий быстро множатся и находят применение в широком диапазоне областей, таких как микробиология, медицина, пищевая промышленность, сельское хозяйство, генетически модифицированные организмы и др. Современные и будущие медицинские технологии базируются на невероятном прогрессе, достигнутом в области нанотехнологий, биотехнологий, получаемой из расшифровки генома человека информации, а также других научных и технических областей. В стадии разработки находятся такие направления: как создание роботов по уходу за больными, интерфейсы " мозг-компьютер", методы целенаправленной доставки лекарств, генная терапия, неинвазивная стимуляция нейронов мозга, роботизированная хирургия, создание биосенсоров и многие другие. Однако, с быстрым развитием биотехнологий возникают и проблемы. Например, исследования с патогенными агентами, такими как вирусы, бактерии, или генетически модифицированные многоклеточные организмы, вызывают беспокойство не только для людей, но и для окружающей среды из-за их потенциальной биологической опасности и мало предсказуемых или недостаточно изученных последствий. В докладе будут представлены достижения и проблемы в развитии современных биотехнологий, а также рассказано о созданных в нашей лаборатории генетически кодируемых биосенсорах и разрабатываемых оптофармакологических соединениях, перспективных для регуляции функций нервной системы человека и животных.

Chernego Daria
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Characteristics of Caregiving Environment in Institutions for Infants Left without Parental Care

SCIENTIFIC ORGANIZATION

Saint Petersburg State University

ABSTRACT

The report will focus on various aspects of social environment to which children growing up without parental care are exposed in specialized institutions in the Russian Federation.

KEYWORDS

Institutionalization, orphanage, caregiving environment.

SUMMARY

Child development is highly dependent on the numerous environmental contexts in which it unfolds, first and foremost, the family environment and, especially, specific facets of childcare and social interactions. According to the attachment theory (Ainsworth, Blehar, Waters, Wall, 1974; Bowlby, 1958, 1969) and the concept of subjective experience development in infancy (Stern, 1985) children need sensitive and responsive caregiver-child interactions with a consistently available caregiver. Institutionalized children experience a lack of opportunity to interact with a caregiver, and their rearing environment is not supportive, sensitive and stable (McCall et al., 2016; The St. Petersburg - USA Orphanage Research Team, 2005; van IJzendoorn et al., 2011). Moreover, research coalesces on the proposition that the quality of child-caregiver interaction has a stronger effect on child development

than nutrition, sanitation and medical care (McCall, 2011; Rutter & Strufe, 2000). Unfortunately, there is a lack of studies to date focused on the relation between the quality of primary environment and the individual developmental trajectory of institutionalized children.

The aim of the current research is to study characteristics of care and social environment for children in institutional care, in different institutional caregiving environments, in order to better understand the complex role of various social environments in the bio-behavioral (behavioral, neurophysiologic and epigenetic) development of children in infancy and early childhood.

This research was supported by grant from Government of Russian Federation #14. Z50.31.0027.

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A potential significance of controlled autophagy in the enhancement of oncolytic virotherapy

SCIENTIFIC ORGANIZATION

Engelhardt Institute of Molecular Biology of the Russian Academy of Sciences

ABSTRACT

Autophagy is an evolutionary conserved process leading to degradation of long-lived proteins, damaged organelles and invasive pathogens. Although autophagy prevents the accumulation of non-functional proteins and organelles thereby reducing the probability of malignant transformation, it may also contribute to tumor growth by promoting cell survival. Autophagy is often upregulated in response to cancer chemotherapy.

KEYWORDS

Cancer, oncolytic viruses.

SUMMARY

Oncolytic virotherapy is a promising approach for the treatment of cancer patients, although more studies is required to increase its clinical efficiency. It is important to explore new strategies to enhance oncolytic properties of viruses. Many viruses have developed a variety of mechanisms that either inhibit the autophagic degradation, or subverts the autophagy process for their own benefit. The aim of this study was to explore the role of autophagy in replication of some oncolytic viruses. Members of non-pathogenic enteroviruses and paramyxoviruses have been chosen for the study. We found that only some of the viruses tested were capable of inducing the autophagy in cancer cells. The induction of autophagy by Torin-2, a direct inhibitor of mTOR was capable of promoting the oncolysis by paramyxovirus Sendai, while some other viruses exploited induced autophagy to prolong virus production by suppressing premature cell death. We suggest that a deliberate modulation of the autophagy may by helpful for the enhancement of oncolytic effects representing a supplemental antitumor strategy.

ADDITIONAL INFORMATION

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Influence of p53 reactivation by RETRA and its novel analogue on the anti-tumour effect of doxorubicin in tumour cells bearing mutated p53

SCIENTIFIC ORGANIZATION

Engelhardt Institute of Molecular Biology of the Russian Academy of Sciences

SUMMARY

P53 family comprises three transcription factors: p53, p63, and p73. p53 is a tumour suppressor protein which participates in many cellular processes and mediates cell response to a wide range of stress stimuli. Its importance for cell quality control is supported by the fact that p53 is mutated in about 50% of human malignant tumours. Mutation of one allele inactivates functional p53 and its siblings p73 and p63 by a dominant-negative mechanism forming oligomers that fail to transcriptionally activate target genes which promote cytotoxic and cytostatic effects. The small molecule RETRA which was identified in our laboratory reactivates p53 family function in cells with mutant p53 following by p73-dependent tumour cell growth inhibition. We designed modifications of RETRA and tested the most efficient analogue (estimated by activation of p53-dependent reporter) for ability to inhibit growth of tumour cells alone and in combination with a routinely-used chemotherapeutic drug doxorubicin since activation of p53-dependent reporter is pronounced at concentrations non-toxic for cells with wild-type p53. This approach may provide a specific elimination of tumour cells with mutant p53 allowing to reduce adverse effects and general toxicity of chemotherapy due to decreased doses of drugs. We are also searching for other combinations of small molecules that may enhance anti-tumour effect of chemotherapeutic drugs in cells bearing both mutant and wild-type p53.

ADDITIONAL INFORMATION

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ACE phenotyping in human heart

SCIENTIFIC ORGANIZATION

University of Illinois at Chicago

ABSTRACT

We performed ACE phenotyping in the human heart. Conformational fingerprint of heart ACE (i.e., the pattern of 17 mAbs binding to different epitopes on ACE) significantly differed from that of lung ACE which reflects differences in the local conformations of these ACEs, likely due to different ACE glycosylation in these tissues. Such difference will be the base for the generation of heart ACE-specific mAbs, that will be used for the development of blood based assay for identification of patients with the increased level of heart ACE (i.e. with the increased risk of atrial fibrillation).

KEYWORDS

Angiotensin I-converting enzyme, heart, atrial fibrillation, lung, conformation.

ACKNOWLEDGEMENTS

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SUMMARY

Background. Angiotensin-converting enzyme (ACE) which metabolizes many peptides and plays a key role in blood pressure regulation and vascular remodeling is expressed as a type-1 membrane glycoprotein on the surface of endothelial cells in the heart and lung.

Methods/Principal findings. We performed ACE phenotyping (ACE levels, conformation and kinetic characteristics) in the human heart and compared it with that in the lung. ACE activity in human heart tissues was 10-15 lower than that in lung. “Conformational fingerprint” of heart ACE (i.e., the pattern of 17 mAbs binding to different epitopes on ACE) significantly differed from that of lung ACE which reflects differences in the local conformations of these ACEs, likely due to different ACE glycosylation in the heart and lung tissues. Substrate specificity of the heart and lung ACEs towards a number of synthetic substrates also differed. Moreover, apparent ACE activity as well as local conformation of ACE in the atria slightly differed from those in ventricles. Various ACE effectors, LMW endogenous ACE inhibitors and HMW ACE-binding partners, were shown to be present in the heart and lung tissues.

Conclusions. **Conclusions**. The significant differences in the local conformations of heart ACE (originated from heart endothelial cells and likely myofibroblasts) and lung ACE (originated from lung endothelial cells) allow us to suggest that the properties and functions of ACE could be sensitive to the microenvironment and be regulated by constituents of tissues and blood, this regulation could depend on a set of possible ACE effectors in heart and lung tissues.

Therefore, significant structural differences in ACE from heart and ACE from lung demonstrated in this study may be the base for the generation of mAbs, which will distinguish these two ACEs. Such mAbs may be used for the development of blood based assay for quantification of heart-derived ACE in the blood for identification of the patients with the increased level of heart ACE (i.e. with the increased risk of atrial fibrillation).

Davydova Aleksandra
Student

Psychophysiological parameters of prosodic discrimination in children with a history of psychosocial deprivation

SCIENTIFIC ORGANIZATION

Saint-Petersburg State University

ABSTRACT

Our study investigated electrophysiological aspects of prosodic processing in children with history of psychosocial deprivation. To test prosodic discrimination we used modified version of experimental paradigm proposed by Grossmann, Striano, & Friederici (2005). During the talk, we will present data collected from children living in different environments, such as children raised in baby homes and their peers from biological families in the age range from 20 to 48 months.

KEYWORDS

Prosody, psychosocial deprivation.

ACKNOWLEDGEMENTS

This research is supported by the grant from the Government of Russian Federation №14.Z50.31.0027.

SUMMARY

During the first several years of life children rapidly acquire basic cognitive and language skills (Rueda, Posner, & Rothbart, 2005). The sensibility and responsiveness of caregiver have been found to facilitate children’s attention (Olson, Bates, Sandy, & Schilling, 2002), cognitive, and language development (Landry, Smith, & Swank, 2006). When caregiver is absent or provides impoverished input, children often exhibit lags in a variety of developmental domains, including cognitive and social-emotional development (Nelson, 2007; Pears, Fisher, Bruce, Kim, & Yoerger, 2010). Institutional environments provide children with suboptimal social and cognitive/linguistic experiences needed to develop basic socio-emotional abilities such as joint attention, face processing, and secure attachment (Плешкова, Мухамедрахимов, 2007). Without these foundational competencies, institutionalized children (IC) have an insufficient basis to acquire more comprehensive

and complicated socio-emotional skills such as reading social cues transmitted through voice and face.

The current study is focused on the electrophysiological aspects of prosodic information processing in children with and without history of early psychosocial deprivation and institutionalization. Linguistic Encyclopedic Dictionary defines prosody as a system of phonetic patterns (pitch, volume, tempo and rhythm), realized in the speech at all levels of speech segments (syllable, word, phrase, syntagm, phrase, text). Prosody may reflect various features of the speaker or the utterance: the emotional state of the speaker; the form of the utterance (statement, question, or command); the presence of irony or sarcasm; emphasis, contrast, and focus; or other elements of language that may not be encoded by grammar or by means of vocabulary.

Unlike the voluminous behavioral work on processing facial expressions in infancy (Parker, Nelson, 2005; Moulson, Westerlund, Fox, Zeanah, & Nelson, 2009), studies on infants' perception of vocal expressions of emotion are scarce, and to the best of our knowledge these abilities have not been examined in children raised in suboptimal caregiving environments.

The body of research on prosodic discrimination in infancy falls into two broad categories depending on the utilized methodology. The first group of methods includes behavioral testing. Habituation paradigm has been frequently used to study prosodic processing in infancy: children are presented with a visual stimulus accompanied by auditory stimulus with prosodic components. After the change of the auditory stimulus, increased looking time to the familiar visual stimulus is taken as evidence of infant's ability to recognize two different vocal expressions. (Walker-Andrews 1983; 1991; Fernald 1988). Studies show that 5 months-old infants can discriminate between happy, sad, and angry vocal expressions by integrating information from visual and auditory domains (Walker-Andrews and Lennon 1991). 5 months-old infants have also been shown to discriminate between happy and sad vocal expressions, when a matching facial expression was presented (Walker-Andrews & Grolnick 1983). 7-month-old infants dishabituated to a change from happy to angry, and from angry to happy emotions, only when both facial and vocal expressions changed, but not when the facial expression was presented alone (Carons, MacLean 1988). Based on this research, a developmental pathway has been proposed in which infants learn to discriminate emotional expressions on the basis of multimodal, vocal, and finally, as visual acuity improves, facial cues (Walker-Andrews, 1997).

The second group of studies utilize electroencephalographic (EEG) and ERP (event-related potentials) methods to study prosodic discrimination in infancy. ERP studies revealed that 7-month-old infants show an increase in a negative component that is thought to reflect the allocation of attention when negative facial expression (fearful) is presented (Nelson & de Haan 1996). 4-month-old infants also have been shown to display more negative shifts in electrical activity registered at the scalp in response to the mother's voice, then in response to the unfamiliar (Purhonen et al. 2004). Words with angry prosody elicited a more negative response in 7-month-old infants' ERPs than words with happy or neutral prosody, which indicates that emotionally charged words undergo more extensive processing than words with neutral prosody (Tobias Grossmann et al., 2005). 7-month-old infants' ERPs are characterized by larger negative component in response to incongruent prosody that mismatched facial expression of the speaker. Conversely, the amplitude of the positive component was larger to emotionally congruent words than to incongruent words (Tobias Grossmann et al., 2006). In 6-10-years-old children's ERPs, N400 component is also attenuated by angry prosody compared to happy and neutral voices (Chronaki et al. 2012). Findings of this study are in line with research conducted with adult participants showing reduced N400 amplitudes to negative compared to neutral emotional stimuli (Kanske & Kotz, 2007).

The brief review of published literature presented above suggests that research on prosodic discrimination in infancy has mainly focused on typically developing children. In our study, we focused our attention on children who are raised in institutional care. To test prosodic discrimination we used modified version of experimental paradigm proposed by Grossmann, Striano, & Friederici, (2005). In this paradigm, children are seated in front of a computer screen on caregiver's lap and watch pictures of a faces (happy, angry and neutral) that are accompanied by auditory stimuli (pseudoword spoken with a different intonation). In different conditions facial expressions and prosodic characteristics either match or mismatch in emotional tone. EEG signal is recorded using a high-density active electrode setup

with actiCHamp EEG system. ERP data was collected from children living in different environments, such as children raised in baby homes (IC) and their peers from biological families (BF) in the age range from 21 to 48 months.

Based on previous research documenting language and socio-emotional deficits in this group, we hypothesize that the ability of children with a history of institutionalization (IC) to discriminate prosodic contour is compromised by impoverished environment of institutional settings and their neural response to prosodic incongruity will be different from that in BF children (raised in biological family). We suggest that the main differences between the IC and BF groups will be found in the processing of negative emotional information. We are currently at the stage of data collection, and will present the preliminary findings at the conference during the talk.

Dvoinina Lublyana
Student

Advanced carriers as ultrafine fibers and laser-treated films

SCIENTIFIC ORGANIZATION

Siberian Federal University

ABSTRACT

In the framework of the project initiated by the Government of the Russian Federation were obtained PHA family as ultrafine fibers and laser-treated films. Experiments showed that laser treatment influenced the surface structure and properties of the P(3HB) films, increasing surface porosity, and improving cell adhesion and proliferation. None of the fibrous scaffolds produced from PHAs had any adverse effects on attachment, growth, and viability of cells. All of them were found to be suitable for tissue engineering applications.

KEYWORDS

Biopolymers; ultrafine fibers; laser-treated films; biocompatibility.

SUMMARY

Advances in science and technology have led to the increasing use of various high-molecular-weight polymer compounds in different fields of medicine. Polymers play a big part in manufacture of high-tech materials and biomedical devices, and in improvement of novel reconstruction technologies. The great diversity of polymers, whose composition, stereoconfiguration, and molecular weight can be widely varied, and the possibility of producing polymer composites with different substances provide a basis for fabricating a very wide range of materials with novel valuable properties.

The most extensively used polyesters for biomedical purposes are polylactides (PLA) and polyglycolides (PGA); in 1970, they were approved by the United States Food and Drug Administration (USFDA) for medical use in the USA. The second most commonly used and comprehensively studied polymers are hydroxy derivatives of alkanoic acids, polyhydroxyalkanoates (PHAs). PHAs are biodegradable, biocompatible, and thermoplastic polymers; PHA-based products are mechanically strong. Poly(3-hydroxybutyrate [P(3HB)] – the most comprehensively studied and commonly used PHA – is not soluble in aqueous media, and, thus, it is biodegraded at a slower rate, producing butyric acid, which does not cause dramatic acidification of the tissues [1–4]. PHAs are promising for constructing biomedical devices, including nonwoven and disposable products, sutures, and wound dressings, controlled drug delivery systems, scaffolds for cellular and tissue engineering, and elements for surgical reconstruction and transplantation [4–9].

Processing properties of P(3HB) can be improved by employing a number of approaches. These are construction of recombinant strains capable of producing PHA copolymers, which incorporate combination of the key genes responsible for the synthesis of monomers of PHA cellular cycle from various microorganisms; creation of special conditions of cultivation and carbon nutrition for wild-type strains to produce polymers with various compositions and improved processing properties – a decreased degree of crystallinity and increased ductility; and construc-

tion of composite materials and blends of P(3HB), and other natural and synthetic materials.

A new approach to the modification of polymer products is to treat them by physical methods or chemical reagents in order to enhance adhesive properties of the surface and facilitate attachment of the cultured cells, to improve gas-dynamic properties of the products, and to increase their permeability for substrates and metabolic products of cells and tissues. Laser treatment is a relatively new approach in the modification of polymer products. Its main advantage over other treatments is that it modifies the surface selectively, without destroying the material or producing toxic substances.

Electrospinning (electrostatic spinning) is a promising technique that can be used for fabricating micro and ultrafine fibers and fibrous scaffolds (mats) and membranes. This technique was introduced in the 20th century to fabricate synthetic fibers. Electrospinning studies using PHAs have not been conducted until quite recently.

The purpose of this study were: to produce electrospun ultrafine fibers differing in their physicochemical properties using PHAs with dissimilar chemical structures and to investigate the influence of electrospinning parameters and PHA chemical composition on the morphology of ultrafine fibers and physical-mechanical and biological properties of fibrous scaffolds; to investigate the effects of different types of laser processing on the structure and physical, mechanical, and biological properties of P(3HB) films.

PHA samples were extracted from bacterial biomass with chloroform and precipitated in hexane. The optimized extraction procedure enabled the production of medically pure specimens that contained no organic impurities (proteins, carbohydrates or lipids, including fatty acids) and were suitable for use in contact with blood [10].

Ultrafine fibers were prepared by electrospinning from high-purity PHA specimens with different chemical structure containing different monomer fractions (3-hydroxybutyric acid, 3-hydroxybutyric and 3-hydroxyvaleric, 3-hydroxybutyric and 3-hydrohexanoic, 3-hydroxybutyric and 4-hydroxybutyric acids).

Ultrafine fibers were electrospun from PHA solutions using a Nanon 01A automatic setup (MECC Inc., Japan). Chloroform solutions with polymer concentration varied from 1 to 10 wt.% were prepared from all types of PHAs. The polymer solution was poured into a plastic syringe (13 mm inside diameter). The syringe was fixed horizontally in the setup, the solution feeding rate varied from 4 to 8 ml/h, the applied voltage from 15 to 30 kV, and the working distance from 11 to 15 cm. Randomly oriented or aligned ultrafine fibers were collected on a flat steel plate or a rotating drum (at 1000 rpm), respectively; both collectors were covered with aluminum foil to collect ultrafine fibers more effectively.

Laser treatment of the surface of flexible transparent polymer films was performed by moderate uniform irradiation of the surface, using CO_2 lasers. In the first series of experiments, polymer films were treated using a LaserPro Explorer II system (Coherent, U.S.), with power varying between 1.5 and 16.5 W and the speed between 0.8 and 2 m/s. Under these conditions, the film surface was uniformly irradiated, and no considerable damage or perforation occurred. The treatment was performed in the focused and defocused modes. In the second series of experiments, films were treated using a LaserPro Spirit system (Sunrad, U.S.) at its highest power, 25 W.

The microstructures of ultrafine fibers and laser-treated films were analyzed using scanning electron microscopy (S-5500 (Hitachi, Japan), and TM 3000 (Hitachi, Japan). Prior to microscopy, the samples were sputter-coated with platinum (at 10 mA, for 40 s), with an Emitech K575X sputter coater.

The effect of the density of polymer solutions on fiber properties was studied using the homopolymer of 3-hydroxybutyric acid, in order to avoid the influence of chemical composition of the PHA on the electrospinning process and properties of the products. P(3HB) chloroform solutions with polymer concentration varied from 1 to 10 wt.% were used. The process parameters were as follows: needle diameter – 1 mm, applied voltage – 30 kV, solution feeding rate – 5 ml/h, and working distance – 15 cm, a flat steel collection plate.

Stable electrospinning of ultrafine fibers in the Nanon 01A setup was attained from P(3HB) solutions with polymer concentrations from 2 to 8 wt.% (solution viscosity 200–800 cP). Polymer concentration significantly influenced the diameter of the ul-

trafine fibers, which varied from 0.45 to 3.14 μm. Within the study range of polymer concentration, the diameter of the ultrafine fibers is linearly related to the solution density. The viscosity of the solutions with polymer concentrations above 8 wt.% was too high (about 1000 cP) to allow successful formation of ultrafine fibers.

We prepared ultrafine fibers using PHAs with different chemical structures and studied the effect of polymer composition on the surface structure and physical-mechanical properties of the fibers. First, electrospun aligned fibrous scaffolds differed from randomly oriented ones in that they had much higher mechanical strength. Second, the effects of the second monomers of the copolymers used to prepare the fibers on the properties of the aligned fibrous mats were different from their effects on the properties of the randomly oriented fibrous mats. The aligned fibrous mats prepared from copolymers containing 3HV and 3HHx had similar values of tensile strength and Young's modulus, and they were not significantly lower than those of P(3HB) fibers, but their elasticity values differed by a factor of two. In P(3HB-co-10 mol.%-4HB) fibers, both parameters characterizing mechanical strength were lower than in P(3HB) ones, but this difference was not as significant as in randomly oriented fibers, while elasticity was more than four times higher.

The most important difference between randomly oriented and aligned copolymer fibrous scaffolds was that in the latter, increased molar fractions of the second monomers had pronounced effect on the properties of the scaffolds.

Biological properties of fibrous scaffolds were studied in the culture of NIH 3T3 fibroblast cells. Investigation of cell attachment and proliferation on scaffolds prepared from solutions of the P(3HB) homopolymer of different densities (2, 4, 6, and 8 wt.%) did not reveal any significant differences at $p \leq 0.05$, showing that all fibrous mats were suitable for use as cell culture scaffolds. At 24 h after seeding, the number of cells on scaffolds was 1.52–1.95 × 10^3 cells/cm^2 irrespective of fiber diameter; at Day 3, the number of cells reached 6.55–8.02 × 103 cells/cm^2. No statistically significant differences were found in the counts of proliferating and viable cells between scaffolds of different types. Hence, the diameter of electrospun P(3HB) fibers did not influence the attachment and growth of NIH 3T3 mouse fibroblast cells.

Thus, MTT assay showed that all PHA fibrous scaffolds facilitated fibroblast cell growth better than the reference scaffolds. Thus, results of MTT assay suggest that all types of fibrous scaffolds facilitate proliferation of fibroblast cells more effectively than the reference scaffolds and that randomly oriented scaffolds are more advantageous for growth and development of this kind of cells than aligned ones.

Results of processing of films using a LaserPro Explorer II system, with the power varied between 1.5 and 12.0 W, corresponding to power density (Q) 0.6 × 104 and 5.3 × 104 W/cm^2, and the speed between 0.8 and 2 m/s are given in Table 1. These treatments did neither cause any considerable damage to films nor generated perforations. The use of a defocused laser beam, with lower radiative flux density, decreased surface deformation.

Measurements of water contact angles on the film surface showed a decrease in this parameter on laser-treated films. In the focused mode, the decrease was more pronounced, and the angle was reduced to 67.4°, while in the defocused mode, it decreased to 79.4°, at the processing speed of 0.8 m/s and 1.8 m/s and power 9 W (or 4 × 104 W/cm^2) and 12 W (0.12 × 104 W/cm^2), respectively. The use of the majority of irradiation modes caused a slight (10–16%) increase in the surface free energy of the film surfaces and a considerable increase (by a factor of 3–5) in its polar component, especially at higher power values. This may suggest that under high-energy impact, new polar functional groups may be generated on the surface and increase the water affinity of the polymer surface.

Changes in surface morphology influence the adhesive properties of the surface and the number of the viable cells attached to it. Fluorescent and electron microscopy of the films with NIH 3T3 mouse fibroblast cells attached to the film surface showed a great number of adherent viable cells. The most highly populated scaffolds were the ones that had been treated at the power and speed of 1.5 W and 1.8 m/s, 3 W and 0.8 m/s, and 9 W and 2 m/s, respectively, in the focused mode, and at 6 W and 2 m/s, respectively, in the defocused mode.

Comparative counts of physiologically active and viable cells cultivated on laser-treated films in MTT assay showed that at day 1, cell counts were similar on all films (about 1.2–1.46 × 10^5 cells/cm^2). At day 4, the number of cells on laser-treated films was greater than in the control. The largest number of viable cells was observed on the films processed by laser radiation at 2 m/s (3.84–5.07 × 10^5 cells/cm^2). The

other scaffolds, including the untreated film (control), had similar amounts of adherent cells: 3.2–3.8 × 10^5 cells/cm^2. At day 7, the populations of cells on scaffolds treated with medium intensity of energy, i.e. 1.5 W/1.8 m/s; 3 W/0.8 m/s; 9 W/2 m/s of focused irradiation and 6 W/2 m/s of defocused irradiation were similar to each other (8.1–8.8 × 10^5 cells/cm^2). These films showed a moderate decrease in the water contact angles (hydrophilicity increase). The number of cells on the films treated with more intensive laser radiation (9 W/0.8 m/s of focused irradiation and 12 W/1.8 m/s of defocused irradiation) was lower – 6.45 and 7.1 × 10^5 cells/cm^2. These results are consistent with the data obtained by microscopy of samples.

Thus, experiments showed that laser treatment influenced the surface structure and properties of the poly(3-hydroxybutyrate) films, increasing surface porosity, and, hence, improving cell adhesion and proliferation.

This study investigated the main parameters of electrospinning of fibers from solutions of PHAs with different compositions that influenced fiber diameter and properties; also polymer products were processed with laser radiation in different modes and tested to find their most promising biomedical uses. The most biocompatible films were produced in experiments with continuous laser treatment, in both focused and defocused modes. Thus, targeted laser modification of films from poly(3-hydroxybutyrate) improves their biomedically important properties. The study revealed electrospinning parameters for the production of high-quality fibers from different types of PHA and determined which parameters should be varied to tailor the properties of the products (fiber diameter, surface morphology, and physical-mechanical properties). None of the fibrous scaffolds produced from PHAs by electrospinning had any adverse effects on attachment, growth, and viability of NIH 3T3 mouse fibroblast cells, and all of them were found to be suitable for tissue engineering applications.

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ADDITIONAL INFORMATION

Study was carried out with the participation PhD student Goncharov D.B. Preferably participate in the poster session.

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Versatile interface framework development

SCIENTIFIC ORGANIZATION

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ABSTRACT

A universal platform for creating devices for the acquisition and processing of biopotentials (EEG, EMG, ECG) is developed. The system is designed to record brain (EEG) or muscle activity (EMG, EKG) and converting the signals into control actions for external devices. Also based on this platform it is possible to create interactive multi-purpose monitors of the state of human health.

KEYWORDS

Versatile framework, BCI, EEG, EMG, ECG.

ACKNOWLEDGEMENTS

This work was funded by the subsidy altocated to Kazan Federal University for the state assignment in the sphere of scientific activities.

SUMMARY

A universal platform for creating devices for the acquisition and processing of biopotentials (EEG, EMG, ECG) is developed. The system is designed to record brain (EEG) or muscle activity (EMG, EKG) and converting the signals into control actions for external devices. Also based on this platform it is possible to create interactive multi-purpose monitors of the state of human health.

The device arranged according to a modular principle and consists of the control communication module and optional remote modules. The control module (CM) based on the STM32F4xxx ARM microcontroller. These microcontrollers allow to vary the computing power and the price of the device without changing the printed circuit board. The CM can operate completely autonomously, powered by its own lithium-ion battery. The CM communicates with the computer via the USB interface with optional galvanic isolation (power and data) module. The CM also acts as a charger (USB) device to the battery. In autonomous mode CM can communicate with the PC, laptop or smartphone via WiFi interface. Also data can be recorded on microSD card.

The interface to the external modules contains: two high-speed serial peripheral interfaces (SPI); digital voltage supply 3.3 V; analog bipolar power-supply ±2.5 V; additional universal input/output ports (UIO). In digital mode the UIO can be used as clock or trigger, in analog mode – like ADC or DAC. It is possible to connect to the CM up to 4 ADC modules with a maximum frequency of digitization.

The overall dimensions of the CM are 6.5 x 5 x 1.5 cm (without shell and battery compartment). The device is supposed under Windows, Linux, Android operating systems; software for MacOS is developed.

At the moment, the converters based on the ADS1298 and ADS1299 are used as remote modules, with the following characteristics:

- ADC resolution 24 bit (provides speed and accuracy of measurements),
- 8 differential or 16 unipolar channels,
- sampling rate 16 kHz (ADS1299, 1 kHz per channel) and 32 kHz (ADS1298, 2 kHz per channel),
- the amplitude of input noise 1 μv (ADS1299), 4 μv (ADS1298),
- programmable gain: 1, 2, 4, 6, 8, 12, (and 24 for ADS1299).

Biopotentials digitization options and the available data transfer capabilities provided by the described device allow to use it both in fundamental research and for clinical needs. The possibility of long-term data collection, including recording to the internal storage, give the potentiality of creation on the basis of the platform detailed diagnostics systems for cardiovascular, neurological diseases or abnormalities of the locomotor apparatus. Also highly configurable remote modules give capabilities for the comprehensive analysis of brain electrical activity (EEG) in the laboratory conditions that is required, for example, during brain-computer interfaces developing.

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Master
Junior Researcher

Synthetic stilbene derivative controls the activity of voltage-gated ion channels of neonatal rat cardiomyocytes

SCIENTIFIC ORGANIZATION

Moscow Institute of Physics and Technology

ABSTRACT

The finding confirms that CTAB-effect on cardiac tissue excitability indeed results from modulation of voltage-gated ion channels responsible for the action potential generation. Thus, the effect of CTAB can be reversed by the washout and is completely irreversible after the UV irradiation. The latter fact gives the opportunity to permanently block the conduction in cardiomyocytes without destroying them.

KEYWORDS

Synthetic Stilbene Derivative, Ion Channels, Patch Clamp, Photocontrol.

SUMMARY

A remote, easily reversible, and precise method for controlling excitable biological tissues, such as heart and neural networks, would have enormous potential for biomedical applications. The modulation of voltage-gated ion channels by azobenzene trimethylammonium bromide (azoTAB) and its influence on cardiac tissue excitability were recently reported. To reduce the toxicity of the photocontrolling substance, stilbene trimethylammonium bromide (CTAB) was synthesized. The structure of stilbene trimethylammonium bromide (CTAB) is very similar to the structure of azobenzene trimethylammonium bromide (azoTAB), with only difference that it is a derivative of stilbene. Presently, we have investigated that CTAB, just like azoTAB, is able to control the excitability of neonatal cardiomyocyte cell culture. *Trans*-CTAB blocks the excitation waves in cultured monolayers of cardiomyocytes. However, there is a significant difference between the action of *cis*-forms of azoTAB and CTAB. The blocking effect of C-TAB remains after UV irradiation (λ~365 nm), when *trans*-CTAB turns to *cis*-CTAB, and stays permanently. The excitability of cardiac cell culture can be restored by washout of the cell monolayers from *trans*-CTAB.

As the membrane potential of cardiac cells is mainly controlled by the activity of voltage-gated ion channels, this study examined whether the sensitization effect of CTAB was exerted primarily via the modulation of the voltage-gated ion channel activity. For this purpose, we performed perforated whole-cell patch-clamp recordings from single ventricular cardiomyocytes, derived from neonatal rats under various conditions (with *trans*- and *cis*- isoforms of CTAB at visible and near-UV illumination, respectively).

The effects of *trans*- and *cis*- isomers of CTAB on voltage-dependent sodium (INav), calcium (ICav), and potassium (IKv) currents in isolated neonatal rat cardiomyocytes were investigated. The experiments showed that CTAB modulated ion currents, causing suppression of the sodium (Na^+) and calcium (Ca^{2+}) currents and potentiation of the net potassium (K^+) currents. We can restore the ion currents by washout cardiac cells from *trans*-CTAB. But after UV-irradiation (λ~365 nm) of the isolated cardiac cells in the presence of CTAB the currents can not be restored. The modulation of the ion channels activity is occurred at a lower concentration of CTAB (60 μM) than concentration of azoTAB (100 μM). This finding confirms that CTAB-effect on cardiac tissue excitability indeed results from modulation of voltage-gated ion channels responsible for the action potential generation. Thus, the effect of CTAB can be reversed by the washout and is completely irreversible after the UV irradiation. The latter fact gives the opportunity to permanently block the conduction in cardiomyocytes without destroying them.

ADDITIONAL INFORMATION

Valeriya A. Tsvelaya, Konstantin Agladze.

Garbuz David
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Recombinant human stress protein Hsp70 as a perspective neuroprotective agent

SCIENTIFIC ORGANIZATION

Engelhardt Institute of Molecular Biology of the Russian Academy of Sciences

ABSTRACT

Molecular chaperone Hsp70 plays protective role in various neurodegenerative disorders. We have shown that exogenous Hsp70 (eHsp70) decreased beta-amyloid level and regenerated neuron density in two mouse models of Alzheimer disease. Futhermore, eHsp70 normalized biochemical parameters in the brain of aged mice. In both cases eHsp70 restored behavior and memory disturbed by Alzheimer disease and aging. The potential of eHsp70 intranasal treatment offers a unique pharmacological approach for various neurodegenerative disorders associated with human aging.

KEYWORDS

Hsp70, Alzheimer disease, neurodegeneration.

SUMMARY

Alzheimer's disease (AD) is the most prevalent neurodegenerative pathology in the growing population of elderly humans and leads eventually to dementia and death. Despite tremendous efforts, no effective treatment for AD is currently available. The severity of cognitive impairment in patients with AD usually correlates with the extent of the observed abnormality of neurons, including the quantity of neurofibrillary tangles, the decrease in synaptic density, the enhanced concentration of soluble Aβ-amyloid oligomers, and the amount of neurons that die by apoptosis (1). Heat shock proteins (Hsps) have emerged as critical regulators of neurodegenerative processes associated with protein misfolding in the brains of AD patients (2). Various data suggest that Hsp70 and other molecular chaperones function as a complex neuroprotective system, which fails in the brains of AD patients. Hsp70 confer protection against oxidative stress and inflammation which play a major role in many age-related pathologies including Alzheimer disease (AD). Despite this, the direct therapeutic effect of exogenous Hsp70 administration on longevity in mammals has not been demonstrated.

To test possible neuroprotective effect of recombinant human Hsp70 we used two separate mouse models of AD-like pathology, bulbectomized NMRI mice and transgenic 5XFAD mice. Bulbectomy in 10-weeks aged mice leads to rapidly development of AD symptoms such as Aβ-peptide accumulation and loss of cortical and hippocampal neurons, and behavior disorders (3). 5XFAD mice co-express the Swedish (K670N/M671L), Florida (I716V) and London (V717I) mutations in human Aβ-PP(695), and M146L and L286V mutations in PS1, with expression of both transgenes driven by Thy1 promoter. This strain is characterized by rapidly neurodegeneration and Aβ plaques formation like in the case of human AD. Sham operated (without bulb aspiration) NMRI or untreated NMRI mice were used as animal control. All mice were treated with Hsp70 (2 ug/mouse in form of intranasal injections) daily for 21 days. Termally denatured Hsp70, physiological solution and bovine serum albumin were used as treatment control for the same time.

We have shown that recombinant Hsp70 expressed in eukaryotic cell cultures as well as in *Escherichia coli* rapidly enters specific brain regions after intranasal administration in mice. We confirmed localization of recombinant Hsp70 conjugated with Alexa Fluor 647 in mouse brains following intranasal injections (Figure 1). The experiments were performed in parallel with iodinated Hsp70 injections. Three hours after administration, fluorescently labeled Hsp70 was readily detected in the hippocampus and temporal cortex in the experimental but not in the control untreated mice (Figure 1). In most cases, the injected protein exhibited intracellular localization, which was concentrated in the perinuclear zone. Finally, intranasally injected fluorescent labeled recombinant Hsp70 observed in brain regions including specific areas (e.g., hippocampus) where neurodegeneration predominantly develops in AD patients and in the process of aging.

To resolve this issue, we decided to use 125I-labeled recombinant Hsp70. We demonstrated that the protein rapidly (within 30 min) enters different brain regions after administration but apparently undergoes rapid proteolysis and is not detectable

in an intact form (70 kD band) after one hour. Labeled BSA, which was used as a control, exhibited similar pattern of penetration and degradation in the brain. These results shown that Hsp70 effectively crosses the blood-brain barrier when administered intranasally.

In the next step we have shown that intranasally Hsp70 treatment reduces the accumulation of Aβ-peptide in the brains of OBX and 5XFAD mice. The total amount of soluble and insoluble fractions of Aβ in the untreated groups of OBX and 5XFAD mice was significantly higher than that in the control and groups subjected to Hsp70 treatment ($p < 0.001$) (Figure 2). Importantly, Hsp70 treatment per se did not affect the basal level of Aβ in the control groups. Thus, Hsp70 treatment effectively protects the brains of mice from the accumulation of potentially toxic Aβ-peptide in both animal models of AD.

It is known that 5XFAD mice develop characteristic Aβ plaques in 2 – 3 months after birth (3, 4). Intranasal Hsp70 administration strongly diminished the plaque density in the neocortex and CA1 region of the hippocampus in Hsp70-treated 5XFAD mice (Figure 2).

Despite the pronounced accumulation of Aβ, OBX mice do not develop plaques, but do demonstrate death of neurons in the brain (4). Therefore, we explored the effect of Hsp70 on neurons morphology and survival in the cortex and the hippocampus of OBX animals. The proportion of pathologic neurons decreased drastically in OBX+Hsp70 animals. The data demonstrate that the Hsp70 treatment prevents the development of pathology in neurons of the OBX group. Consistent with the protection of cells, Hsp70 significantly improved neuronal survival in OBX mice. Quantitative analysis revealed that the Hsp70-treated OBX mice had significantly more intact neurons in the temporal cortex and hippocampus. Therefore, Hsp70 treatment of OBX mice protects neurons from deterioration and death in brain areas most affected in AD patients.

Exogenous Hsp70 protects spatial memory decreased in OBX and 5XFAD mice in Morris water maze test. It is evident that untreated OBX and 5XFAD mice had severely impaired spatial memory. In contrast, OBX and 5XFAD mice treated by Hsp70 displayed a significant preference for the target sector. We therefore conclude that subchronic intranasal injection of Hsp70 protected spatial memory in both OBX and 5XFAD animals.

In conclusion, we can summarize that the intranasal administration of recombinant human Hsp70 drastically alleviates all symptoms, including memory loss, neuronal death, cellular aberrations, and accumulation of the Aβ-peptide in both AD-models explored.

In our experiments we also examined whether the intranasal administration of exogenous recombinant human Hsp70 can promote longevity in male and female

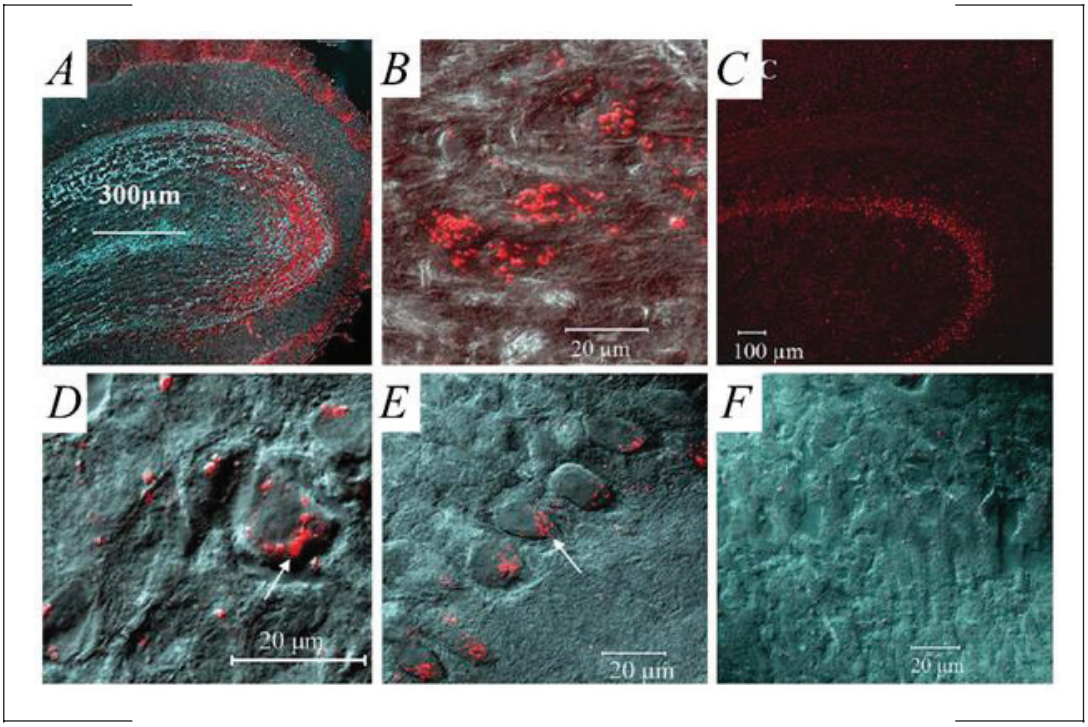

Figure 1. Distribution and stability of recombinant Hsp70 after penetration into the brain of NMRI mice. (A – olfactory bulbs, B – n. raphe dorsalis, C, D – hippocampus, E – cerebellum). Localization of the label in the perinuclear region is indicated by white arrows. F – control mice (injection of unlabeled Hsp70).

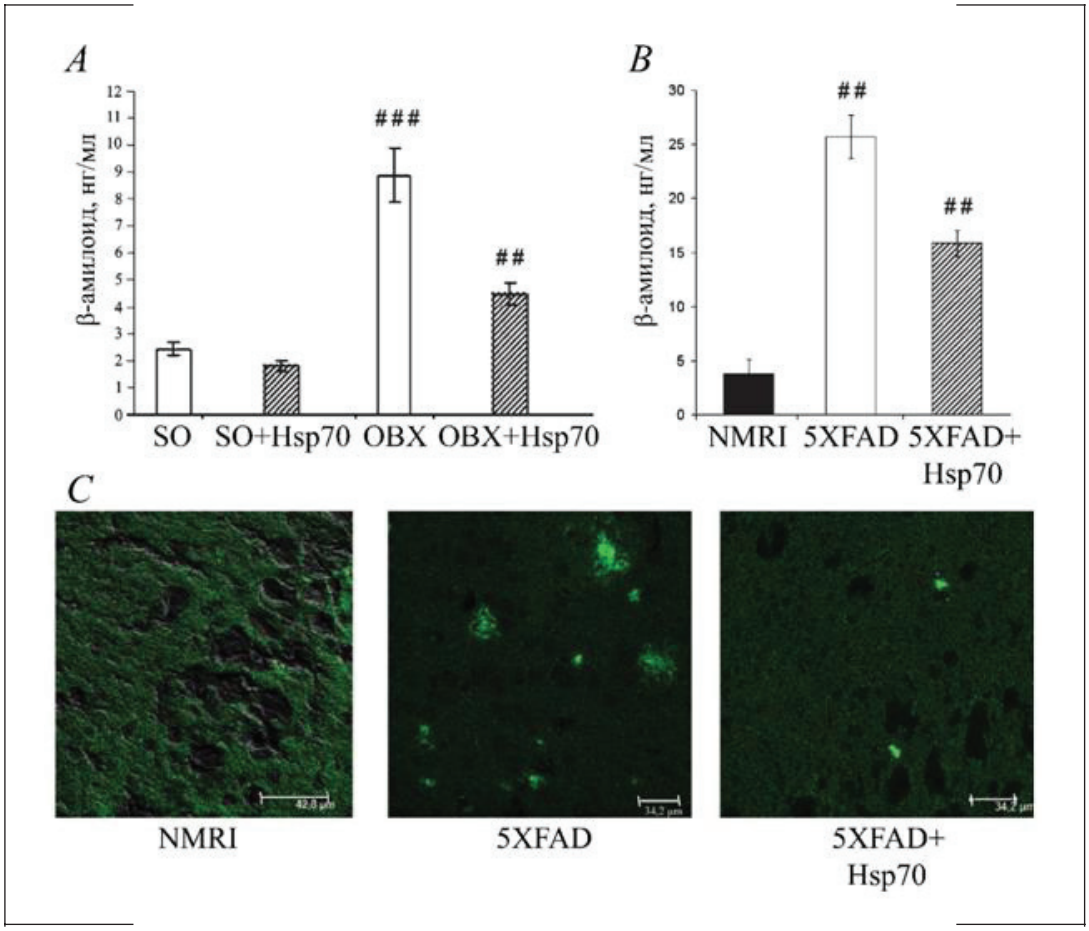

Figure 2. A, B – the level of β-amyloid in the brain of mice: a sham-operated (SO), bulbectomized (OBX) NMRI strain and transgenic 5XFAD, control and subjected to intranasal injections of recombinant Hsp70 (+Hsp70). C – the density of amyloid plaques in 5XFAD mice without Hsp70 treatment and after Hsp70 injections. Micrograph of a slice of NMRI mouse brain is given as the example of a negative control (without the formation of β-amyloid plaques). ## $p \leq 0.01$; ### $p \leq 0.001$.

mice. Interestingly, long-term (chronic) introduction of Hsp70 did not affect the longevity of females significantly, while increased the lifespan of males (Figure 3). The Hsp70 treatment also normalized the synthesis of synaptophysin and decreased accumulation of lipofuscin which represent the marker of aging and neurodegeneration processes (Figure 4).

We hypothesized that Hsp70 exerts its protective effects on behavior by decreasing the production and/or accumulation of damaged proteins in the brain. A majority of intracellular proteins are degraded by proteasomes; thus, the catalytic activity of proteasomes is critical to the homeostatic process. Because proteasome activity decreases with age in brain (5), we investigated whether eHsp70 treatment altered proteasome activity in the brains of treated mice. Caspase-like activity in the cortices of control animals was comparable to that detected in brains of Hsp70-treated mice. In contrast, chymotrypsin-like activity in mice of the Hsp70-treated group was significantly increased. We analyzed the subunit composition of proteasomes

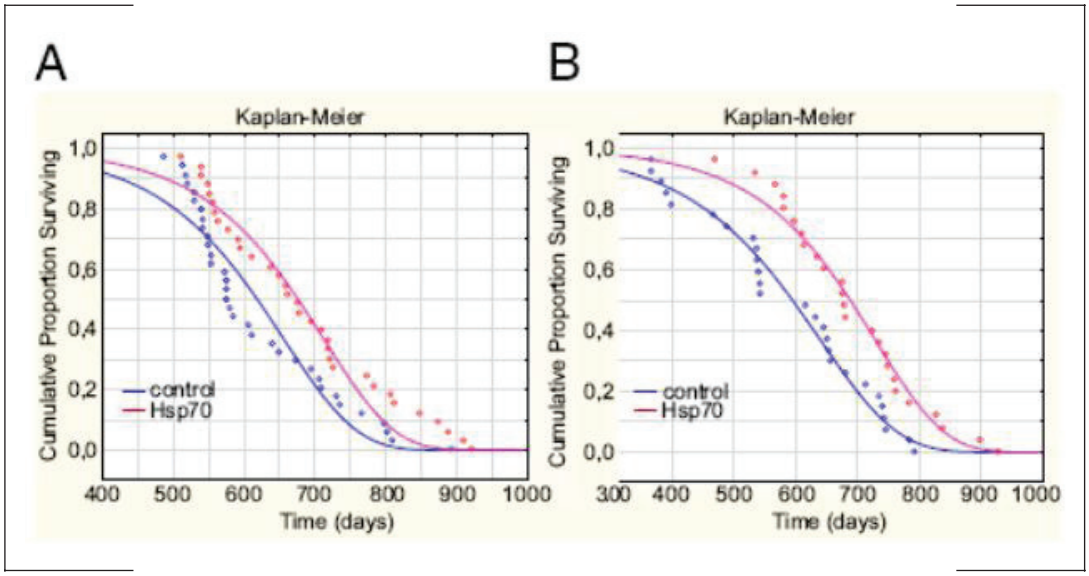

Figure 3. Effect of chronic eHsp70 treatment on longevity. (A) Longevity of old animals when Hsp70 treatment was started at 17 months of age and lasted until animals' death. (B) Longevity of middle-aged animals when eHsp70 treatment was started at 12 months of age and lasted until animals' death.

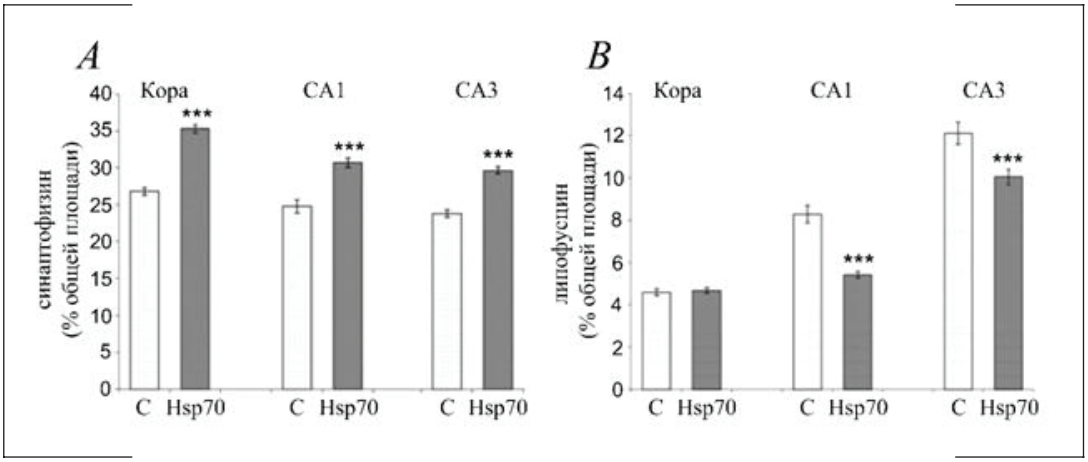

Figure 4. Effect of eHsp70 administration for 5 mo on molecular markers of aging. Levels of synaptophysin (A) or lipofuscin (B) were measured in the brains of Hsp70-treated and control old mice. *** $p \leq 0.01$.

after intranasal Hsp70 injections and observed a significant elevation in the Rpt6, β6 and β5i subunits expression. These findings suggest that the elevated chymotrypsin-like activity in the brains from eHsp70-treated animals is likely due to the increased amount of proteasomes containing the β5i subunit.

In parallel with effects on biochemical level Hsp70 treatment leads to increasing of neuronal density and repairs spatial memory loss in aging mice as well as in AD models (OBX and 5XFAD).

Taken together, our findings establish exogenous human Hsp70 as a practical pharmacological agent for the treatment of various neurodegenerative diseases (as well as the consequences of brain injury) and possibly aging.

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ADDITIONAL INFORMATION

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The mechanisms of Drosophila spindle assembly: The role of kinetochore-driven microtubule formation

SCIENTIFIC ORGANIZATION

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ABSTRACT

We analyzed the molecular mechanisms of mitotic spindle assembly in Drosophila S2 cells. Using a combination of RNAi-mediated protein depletion and microtubule (MT) regrowth assays after MT depolymerization, we identified a number of factors that affect kinetochore driven MT assembly. Our results provide novel insight into the molecular mechanisms of this process and suggest a model for its regulation.

KEYWORDS

Drosophila S2 cells, mitosis, spindle, kinetochores, microtubule regrowth assay.

SUMMARY

The spindle is a complex and highly dynamic microtubule (MT)-based molecular machine that mediates precise chromosome segregation during both mitosis and meiosis. To form a spindle, centrosome-containing cells exploit 3 classes of microtubules: MTs nucleated by the centrosomes, MTs nucleated near the chromosomes/kinetochores and MT nucleated from preexisting MTs through the augmin-based pathway. Here we report our studies aimed at the identification and characterization of the genes/proteins required for kinetochore-driven MT growth. To identify these proteins we used *Drosophila* S2 cells and determined their proficiency in the process by analyzing spindle MT regrowth after cold- or colcemid-induced MT depolymerization.

We first asked whether the depolymerization conditions affect the pattern of MT regrowth. As expected, we found that after cold treatment MTs regrow much more rapidly than after colcemid treatment. In addition, we found that cold-induced MT disassembly at very low temperatures (-2°C) destroys kinetochore-driven but not centrosome-directed MT regrowth, while MT depolymerization at 0°C allows regrowth from both kinetochores and centrosomes. Colcemid-induced MT depolymerization strongly impaired centrosome-dependent MT nucleation but allowed MT regrowth from kinetochores. These results indicate that the kinetochore- and the centrosome-mediated MT assembly pathways exploit molecular mechanisms that are at least in part different.

We next focused on the cellular functions required for kinetochore-driven MT regrowth, and examined this process in prometaphases/metaphases from cell cultures depleted of specific spindle proteins by RNA interference (RNAi). These analyses identified several factors that positively affect the process (Eb1, Mast/Orbit, Mars, Mei-38 and Dgt6), as well as factors that appear to delay regrowth from kinetochores (Asp and Patronin). These results provide novel insight into the molecular mechanisms of kinetochore-driven MT growth and suggest a model for the regulation of the process. We are currently integrating these studies with in vivo observations of dividing cells expressing Cherry-tagged tubulin or other fluorescently labeled proteins involved in MT regrowth from kinetochores. We are also using transmission electron microscopy to characterize normal mitosis and MT regrowth in S2 cells.

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Using next generation sequencing data for improvement of eukaryotic gene prediction

SCIENTIFIC ORGANIZATION

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ABSTRACT

Genome annotation is vital for most genomic analyses. Still the quality of many annotations of eukaryotic genomes remains poor. Two major approaches to annotation rely on HMM ab-initio prediction or on transferring some existing annotation based on homology. Both have drawbacks. Approaches which combine ab-initio prediction with hints from experimental data (mostly, next generation sequencing data) can greatly improve annotation. I will discuss this method and demonstrate the results obtained with our annotation pipeline on genomes of several plant species.

KEYWORDS

Next generation sequencing, RNA-seq, genome annotation, gene prediction, gene model.

ACKNOWLEDGEMENTS

Grant of Ministry of Education and Science # 11.G34.31.0008, grant of Russian Science Foundation # 14-50-00150.

SUMMARY

Being a basic step in most NGS projects annotation is still very inaccurate. For most de-novo annotations ab-initio prediction is used. The method is based on HMM or machine learning algorithms and attempts to output the most probable gene annotation with respect of the gene model given. Still gene models are often far from being close to biological reality and rarely rely on such things like signaling sequences. The reason is that nature of such signals is often poorly understood (tss, tts) and some of the signals are very smooth (like Kozak sequence or an enhancer). Modeling such signals is not possible. But some hints can be made from experiments like RNA-seq. Mapping the reads from RNA-seq can precisely locale the intron boundaries, detect transcribed regions and determine the proper DNA strand for gene model. Using such hints it is possible to improve the annotation quality significantly. Here we discuss our pipeline which is able to combine hinted ab-initio approach with homology-based scoring system for concurrent gene models. The results of this pipeline usually are of better quality if compared to most widely used methods. We also will discuss the importance of annotation in whole-genome studies and connection between genome assembly and annotation quality.

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Quantification and visualization of HER2 protein using nanocrystals conjugated with single-domain antibodies

SCIENTIFIC ORGANIZATION

Moscow Engineering Physics Institute

ABSTRACT

At present, three classes of fluorescent labels are used for biomedical applications. These are heterocyclic molecules, fluorescent proteins, and photoluminescent (PL) semiconductor nanocrystals or quantum dots (QD). The main advantages of QDs are an extremely high resistance to photobleaching, high PL quantum yield, and continuous range of emission spectra from the ultraviolet to the infrared region depending on the QDs' size. In this study, HER2 protein was visualized and its content was estimated using single-domain antibodies conjugated in a site-specific manner with QDs.

KEYWORDS

Quantum dots, QD; near infrared, NIR; single-domain antibody, sdAb; HER2 protein.

ACKNOWLEDGEMENTS

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SUMMARY

Development of new fluorescent-based visualization is increasing in geometric progression, since fluorescent labeling of macromolecules has become one of the most widespread methods of imaging in modern biology and biotechnology (Fili and Toseland, 2014). The most common fluorophores for biolabeling are low-molecular-weight heterocyclic organic molecules. This type of fluorophores is characterized by a wide range of emission spectra, but their fluorescence is susceptible to photobleaching. Fluorescent proteins, such the widely used green fluorescent protein (GFP), have a higher photostability than heterocyclic molecules, and, in addition, intriguing properties of photoinduced shift of fluorescent emission spectra (Ando et al., 2002) and generation of reactive oxygen species (Wojtovich and Foster, 2014). Nevertheless, some difficulties with producing proteins with infrared fluorescence pose obstacles to their wider applications.

The third type of fluorescent labels includes photoluminescent (PL) semiconductor nanocrystals or quantum dots (QDs). QDs are synthesized from elements of groups IV–VI, such as Cdor Te. Absorbing UV/vis light, QDs emit fluorescence in the form of a narrow peak at wavelengths directly proportional to the QD size (Bruchez Jr., 1998). Due to the continuous variation of the emission maximum, it is possible to obtain nanocrystals with desired emission characteristics. Another useful feature of QDs is their extremely high resistance to photobleaching (Hardzei et al., 2012). The high stability of fluorescence makes QDs very interesting for labeling macromolecules in studying bioprocesses *in vivo* (Lim et al., 2015; Samanta and Medintz, 2016; Tu et al., 2016).

Near-infrared light (NIR) is very weakly absorbed by tissues of living organisms in comparison with UV or visual electromagnetic waves; that is why this region of the optical spectrum is the most promising for bio-imaging. The second attractive feature of IR radiation is its harmlessness for living systems. That is why the use of fluorescence in the IR region of the optical spectrum is considered a very promising approach to biomedical imaging (Song et al., 2016).

In the present study, we have prepared a PL nanoprobe for imaging of human epidermal growth factor receptor 2 (HER2), a very important prognostic marker for cancer diagnostic and treatment (Hadi, 2015; Harris et al., 2007). For the detection of HER2 protein, we have conjugated QDs with a maximum of emission spectra at 570 nm, as well as NIR-light-emitting QDs, with single-domain antibodies (sdAbs) against HER2 protein.

We have developed ultraminiature nanoprobes consisting of highly affine sdAbs or “nanobodies”, which are the smallest possible functionally active antibodies (13 kDa), conjugated with QDs in a strictly oriented manner. The highly ordered orientation of sdAbs on the QD surface is ensured by site-specific conjugation via an additional cysteine residue attached to the C-terminal region of the sdAb amino acid sequence. Each nanoprobe contains four sdAb molecules attached to a QD in the same orientation relative to its surface and has a hydrodynamic diameter smaller than 12 nm.

We present here our results of ELISA quantification of HER2 protein with anti-HER2-QD conjugates and *in situ* visualization of HER2 protein on the surface of HER2-positive cells.

When further validating the flow cytometric detection of cancer markers using QD–sdAb conjugates, we experimentally demonstrated that all other QD–sdAb conjugates obtained were highly specific and could be used to differentially detect very small relative numbers of cancer cells (Figure 1). Experiments with mixtures of human breast cancer cells expressing HER2 (the SK-BR-3 cell line) stained and not stained with conjugates of QDs with anti-HER2 sdAbs, as well as human epidermoid carcinoma cells (the A431 cell line) stained and not stained with conjugates of QDs with anti-EGFR sdAbs, in different ratios showed strong correlation between the numbers of cells identified as HER2- and EGFR-positive and the actual numbers of the respective labeled cells in the mixtures. It proved possible to detect

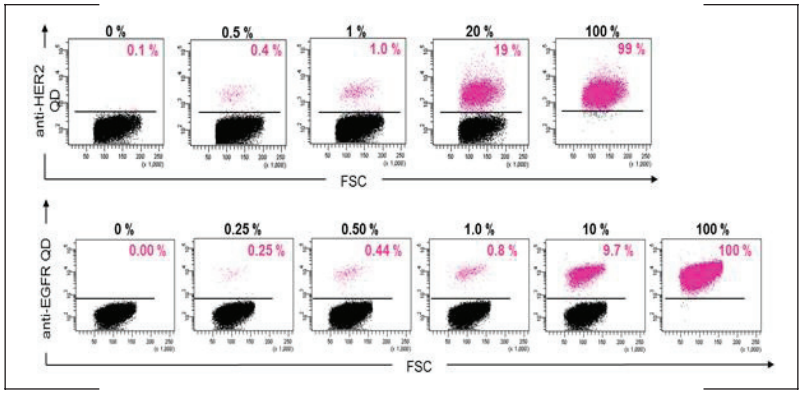

Figure 1. Testing of conjugates of quantum dots (QDs) with single-domain antibodies (sdAbs) against HER2 and EGFR. SK-BR-3 cells stained and not stained with conjugates of QDs and anti-HER2 sdAbs (the upper row) and A431 cells stained and not stained with conjugates of QDs and anti-EGFR sdAbs (the lower row) were mixed in specified ratios. 10^5 cells were incubated in the presence of conjugates containing QD_{570} (30 μg/ml) for 1.5 h at 4°C in a final volume of 50 μl. Immediately after the last washing stage, the ratio between stained and unstained cells was determined using flow cytometry. The numbers above the plots (black) show the actual, prespecified percentages of stained cells; the numbers in the upper right corners of the plots (pink), the estimated percentages of stained cells.

as small proportions of labeled cells as 0.5 and 0.25% among SK-BR-3 and A431 cells, respectively.

The results of our research allow us to propose a method for fabricating QD-based nanoprobes with advanced functional characteristics, including an enhanced sensitivity. Thus, the ultraminiature QD–sdAb nanoprobes with highly ordered orientation of the Ab molecules relative to the QD surface developed in our studies have numerous implications for advanced integrated diagnostics.

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Emotions in institutionalized young children with special needs

SCIENTIFIC ORGANIZATION

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ABSTRACT

Emotions are biological basis and the main source of infants development. Children with special needs (SN) may show unusual emotions and not recognize parent's emotional feedback. The most vulnerable group are SN children in institutions. Investigations demonstrate a positive impact of early intervention programs on development of SN children. But there is a lack of research data on characteristics of emotions in SN children (especially institutionalized) that could help to understand the trajectory of the emotional development and create congruent early intervention programs.

KEYWORDS

Children, special needs, emotions, institutions.

SUMMARY

Introduction

From the beginning of the 19th century develops the idea stated by C.Darvinom that ability of the person to express the emotions is congenital and caused by evolution.

Most often investigated implications are:

- Expressions of emotions on the face
- In a voice
- And as impulses to physical action.

Innateness of all parameters set forth above does not mean that training, education and other factors of environment do not render any influence on expression of emotions by a person.

Izard K. has stated the idea about step-type behaviour of emotions, has underlined their social nature fixed during evolution at level of a biological reflex (Izard, 1977).

External determinants can essentially bedevil the implications of emotions put initially. However the identical character of expression of each emotion repeatedly proved to be true cross-country - cultural researches.

Since the birth the child is capable to express emotions on the face, character of these expressions gradually develops during human life. All muscles of the face which are necessary for expression of various emotions, are formed in fetal development. Therefore the child since the birth is capable to express various emotions which are differentiated subsequently. (Muhamedrahimov, 2008, p.13).

Emotions are the biological basis and the main source of an infant's development. Multiple researches showed that biological reasons and social environment can influence children's ability to recognise and generate emotional expressions.

True recognition of a facial expression of other person, effective utilisation of emotional expressions in interaction become the major skills of the baby. (Caron, Caron, and Myers, 1982; de Haan and Nelson, 1998; Kestenbaum and Nelson, 1990; Ludemann and Nelson, 1988; Nelson, 1987; Nelson and Dolgin, 1985). The human face is special object strong emotional tie with which is pledge the normal physical, cognitive, social and emotional development. (Vinnikott, 2007; Lafreniere, 2004; Stern, 2001; Feldman, 2007; Tronick and Reck, 2009).

For our research it is important to understand evolutionary reasons of occurrence of emotions very important. On a course of evolution of the person the growing period was enlarged, collected experience which it was necessary to transfer to young generation, by means of training. It is important for child's survival, that there should be a close mutual attachment, between him and the person caring of it, there should be a close mutual attachment. The emotions ate the factor of mutual attachment of mother and the child. This social communication between mother and the child has been obliged to be generated during evolution. Another reason of occurrence of emotions was need of communication between mother

and the child, as well as between adult people. It is obvious, as before the occurrence of speech, emotion was the major channel of communications. Emotional communication has enormous value as without it such close interaction between mother and the child would be impossible.

From here follows the importance of early experience of the baby. It is extremely important to establish strong and reliable links between mother and the child which are put since the very first days and even hours of his life. Quality of this links provides normal physical, cognitive, social and emotional development.

Unfortunately, in reality it often happens when due to any reasons the interrelation between mother and the child cannot be established.

Among factors menacing the establishment of effective links mother-child can be defined:

1. The situation of deprivation.

The situation of deprivation deprives of the child of possibility to pass gradually and consistently to pass all stages of communication with mother and gradual possibility to be separated from her.

Since almost biological unity with mother, indissoluble contact to object of attachment, veneering of the general representations about availability and responsiveness of the trustee, up to a stage on which the child is found out the readiness to leave the close adult on short time intervals.

It is important to understand in what surroundings turns out a child who has lost parent care. There is voluminous literature about the researches devoted to a social environment of babies in children's homes. Researchers do a conclusion that only physical needs are satisfied, whereas the psychological are ignored. (Muhamedrahimov, 2008).

Socially caused possibilities to train appearance of emotions in interaction with the close adult are essentially lowered.

There is the rich research material describing consequences of staying in establishment for emotional development of children. (Provence, Lipton, 1991; Muhamedrahimov, 1991, 2003,2008)

- There is a mass of problems with recognition and understanding of emotions with the children deprived of parent guardianship. The special attention is deserved by association between difficulties in emotional processes and the enlarged risk of development of various psychological disorders at such children.

- Children with experience of deprivation distinguish emotions less often correctly distinguish emotions, than usual.

- Children demonstrate difficulties in difference definition between emotional conditions.

- They see more similarities between the happy and sad person, than children in other groups.

- Such children have less possibilities of training to emotions

2. Delays, features of development, physical inability of children can prevent development of emotional mutual understanding between parents and children. (Hyche, Bakeman and Adamson, 1992; Lorraine F. Kubicek, Karen Riley, Jeanine Coleman, Gloria Miller and Toni Linder 2013; Eric Emerson and Stewart Einfeld, 2010).

The given problem can be solved by two approaches. On the one hand, features of emotional expressions, reaction and recognition of emotions can arise because of the general features of development. This point of view has a lot of contradictions, but there are the researches specifying that emotional development, becomes a certain support of the general development of the retarded children, or when a child suffers from physical inability, leaders to problems in informative, behavioural and social spheres. There also programs for children with disorders of an autistic spectrum, a mental retardation, the arrests of development, informing on achievement of results in ability of recognition of emotions at such children.

But as it is necessary to remember that, unfortunately, parents and children with special needs often face problems of behaviour and vital stress factors which can prevent development of high-grade interaction.

The facial expression of children with special requirements can be less expressive and is clear, and answers of parents can be perceived not truly.

Children with special needs (SN) may show unusual emotional reactions and not recognise parent's emotional feedback. The most vulnerable group are children with special needs living in caretaking institutions. (Charles A. Nelson, 2005; Seth D.Pollak, Dante Cicchetti, Katherine Hornung, Alex Reed, 2005; Freedman, Insel, AND Smith, 2000).

Consequences of these factors of the given early experience is indisputable for the child fad leave its mark on all life.

Research shows a positive impact of early intervention programs on development of SN children. But there is a lack of research data on characteristics of emotional expressions manifested by SN children (especially institutionalised) that could help to understand the trajectory of their emotional development and create congruent early intervention programs. (Downs et al., 2008; the Command of researchers of children's homes: St.-Petersburg, the Russian Federation - Pittsburgh, the USA, 2013).

It is obviously important for us to investigate this question from a position of studying of expression of discrete emotions in a situation of immediate interaction of the child and the close adult.

Method

There are many researches in which sample were formed on the basis of medical diagnoses. More often the features of emotional development in these works were considered within the limits of one concrete disturbance.

We tried to consider but not to concentrate on medical indications.

Participants included children with special needs aged 9 to 44 months old from two types of institutions: family-type orphanages and traditional orphanages with deprivation conditions. Children had different medical diagnoses and were combined in the same research group according to the Functional Abilities Index (Simeonsson AND Bailey, 1991; Muhamedrahimov, Palmov, Istomina, 2000).

The technique includes 9 areas of development:

- Hearing
- Behaviour and social skills
- Intellectual functions
- Motor functions
- Orientation on dialogue
- Muscular tone
- The general state of health
- Eyesight
- Anatomical organization

Children's facial emotional expressions were measured using Dyadic Affect Manual (Osofsky, Muhamedrahimov, Hammer, 1998) in a set of episodes: free play child-caregiver interaction - separation - reunion.

The main aim of the technique is to estimate qualitative and quantitative characteristics of emotion on a child's face in the course of interaction with the adult. And evaluate characteristics of emotional reaction of adult interaction in a situation with the child.

Video recording of five three-minute episodes of interaction of the child and the close adult with the subsequent estimation of 8 emotions taking into account their intensity is made.

1 Free game
2 The Adult leaves a room; the child remains one (the first separation)
3 The Adult comes back (the first reunion)
4 The Adult again leaves a room (the second separation)
5 The Adult comes back (the second reunion)

In each situation on a 5-ball scale 8 emotions are estimated: 4 positive (pleasure, interest, excitement, surprise) and 4 negative (grief, sorrow, anger, fear).

Positive and negative emotional tone is calculated. In addition the technique allows to fix indicators of big and small motor function and deadaptative behaviour. Specially trained commission of experts do analysis of video recording.

Results

The Experiment aims to observe emotional manifestations and activities of an infant in various situations during interactions with adults (shown most clearly in stress). Separation from a familiar adult is a major stress-producing factor. SN children out of traditional orphanages differ from those of family-type orphanages in the use of stress-coping techniques. Traditional orphanage children demonstrate a higher positive affect as compared to the second group (M=5,50±2,17 and M=3,55±1,81 accordingly, p=0,003) and a higher motor activity (M=7,40±1,17 and M=6,00±0,41, p=0,04).

Conclusion: Positive affect and motor activity cannot be deemed an adequate stress reaction. Most likely, a hyperbolized elation demonstrated by an infant appears to be false, whereas hyperactivity helps reduce the emotional tension caused by stress. We assume that the above-mentioned strategy can be deemed adaptive within a traditional orphanage and enables an infant to attract an adult's attention in a more efficient manner, than demonstrating true emotions - a strategy that cannot facilitate normal infant development.

The further direction of our study is the decision of a question about differentiation of children with various combinations of safe functional abilities on groups and comparison of characteristics of their emotional reaction to those at typically developing children in children's homes of traditional and family type. We assume that it is possible to achieve the development of strategy of the emotional reaction of children with the established medical diagnosis comparable to those at children of standard group of development of functional abilities. Quality of emotional development of the child with special needs depends on characteristics of its interaction with the close adult, abilities of the adult to see, distinguish and to react to signals of the child with special needs. We consider that results of work will help to develop support programs for children with the special needs, aimed at their harmonious development, both with children's homes, and in families (biological and replacing).

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TNF expression studied with fluorescent reporter system in vitro and in vivo

SCIENTIFIC ORGANIZATION

Lobachevsky State University of Nizhni Novgorod - National Research University

ABSTRACT

Molecular imaging techniques to study TNF expression in autoimmune pathologies may be useful for disease mechanisms studies. Here we utilized protein sensors composed of a single-domain antibody against TNF and far-red fluorescent protein Katushka to evaluate expression levels and localization of this cytokine in disease. Such proteins were expressed in bacterial system, purified, and their functional activity was characterized. In parallel, we used TNF reporter mice to visualize TNF expression in organs and tissues.

KEYWORDS

TNF, VHH, nanobodies, reporter mice, fluorescent sensors, in vivo imaging.

ACKNOWLEDGEMENTS

This work was supported by the Russian Ministry of Science and Education (grant №14.Z50.31.0008), Russian Science Foundation (grant №14-50-00060) and The Russian Foundation for Basic Research (grant №16-34-00561).

SUMMARY

Tumor necrosis factor (TNF) is a pro-inflammatory and immunoregulatory cytokine that plays an important role in protection against pathogens. However dysregu-

lation and excessive TNF production may cause autoimmune and inflammatory pathologies. Study of TNF biology in disease may play an important role in understanding disease mechanisms. Fluorescent imaging provides an opportunity to visualize components of the immune system *in vivo*. One of the most common approaches for the *in vivo* imaging is utilization of fluorescent proteins that are bound or fused to the target molecule, or are co-expressed with it. Fused fluorescent proteins composed of the single-domain antibody against TNF and the red fluorescent protein Katushka might be used for evaluation of expression levels and localization of TNF production [1]. In this study we used two genetic constructs encoding fluorescent proteins VHH41-kat and VHHAnti-hTNF-kat. VHH41-kat protein is able to bind TNF, whereas the protein VHHAnti-hTNF-kat not only binds but also neutralizes the biological activity of TNF.

The first aim of this study was to identify the optimal strain of *E. coli* to produce antibodies VHH41-kat and VHHAnti-hTNF-kat. The expression levels of antibodies in the following *E. coli* strains: Rosetta 2 (DE3) pLysS, BL21 (DE3), BL21 Codon Plus (DE3), Lemo21 (DE3) and B834 (DE3) were compared. The BL21 (DE3) was chosen as the most appropriate *E. coli* strain for production of the studied proteins.

To measure the blocking activity of fused fluorescent proteins *in vitro* the cytotoxic MTT-test with mouse fibrosarcoma cell line WEHI 164 was used. Recombinant human TNF was added to the cell culture at the concentration 200U/ml. Serial dilutions of tested proteins were added to the cell culture in concentration range from 2pM to 1μM per well. Commercial TNF blocker Remicade was used as a control. According to these measurements fluorescent blocker VHHAnti-hTNF-kat possessed a strong anti-TNF activity (LD50 = 3917 pM), while VHH41-kat did not.

To test the ability of VHH41-kat and VHHAnti-hTNF-kat to bind macrophage TNF, the cytofluorometric analysis was performed using bone marrow derived macrophages (BMDM) from humanized TNF mice. Macrophages were activated by LPS (100 ng/ml for 4 hours) in the presence of Brefeldin A and stained for TNF using intracellular cytokine staining protocol. The cytofluorometric analysis showed that both fluorescent antibodies were able to bind TNF produced by macrophages. The fluorescence intensity of VHHAnti-hTNF-kat was higher than the fluorescence intensity of VHH41-kat. Thus, VHH41-kat antibody might be used as a marker of TNF production, and the antibody VHHAnti-hTNF-kat may be considered as a theranostics agent due to its high fluorescence intensity and the ability to block TNF.

To evaluate the blocking activity of the fluorescent proteins in vivo experimental model of acute hepatotoxicity in the humanized mice was used.

Mice that were injected intraperitoneally (i/p) with 150pM/g and 300 pM/g of VHHAnti-hTNF-kat 30 minutes after i/p injection of LPS and D-galactosamine (400 ng/g and 800 μg/g, respectively) remained viable until the end of the experiment (24 hours). In the group of animals receiving the lowest dose (75 mg/g) a partial mortality was observed.

Mice that were injected with 150pM/g and 600 pM/g of VHH41-kat or PBS (as a control) died 6 hours after LPS and D-galactosamine administration. Partial lethality was observed in the group which received 300pM/g of VHH41-kat. Thus, VHHAnti-hTNF-kat at 150 pM/g provides 100% protection of mice.

In a parallel *in vivo* approach we used transgenic “reporter” animals which are able to endogenously co-express TNF and the reporter protein. Specifically, in the reporter TNF-2A-Kat mice immune cells produced red fluorescent protein Katushka under the control of regulatory sequences of the TNF gene. This model allows to follow TNF expression by fluorescent *in vivo* imaging and can be used for detailed study of TNF physiological functions in normal conditions and in TNF-dependent pathologies [2]. Embryos were analyzed on the 17th day of gestation. Analysis of the fluorescence signal of newborns was performed for three days after birth.

Fluorescent analysis of embryos, adult healthy animal organs and newborns of TNF-2A-Kat reporter mice and wild type mice did not show any difference in the intensity of tissue fluorescence. The lack of significant differences was presumably due to the absence of microbiota.

On the contrary, the analysis of TNF production in the adult healthy TNF-2A-Kat reporter mice clearly showed tissue fluorescence presumably due to skin microbiota. Antibacterial drug Neosporin® was applied to the open skin area on the left shoulder of adult TNF-2A-Kat reporter mice and wild type mice for 9 days. A statistically significant difference in fluorescence intensity between normal skin area and the site of Neosporin® application was detected. We concluded that skin microbiota

contributes to constitutive levels of TNF expression in adult healthy TNF-2A-Kat reporter mice.

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SCIENTIFIC ORGANIZATION

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A millennium of research on children growing up without their biological parents: What have we learned and how did we shape the policy?

ABSTRACT

In this presentation, Professor Grigorenko will focus on the current state of knowledge regarding major threats to the development of children growing up without their biological parents in different environments, namely different types of replacement families and institutions. Professor Grigorenko will provide an overview of the literature and particularly highlight aspects that are directly related to the research conducted by her Laboratory at SPbGU.

KEYWORDS

Child, development, physical, cognitive, social-emotional.

ACKNOWLEDGEMENTS

This research was supported by grant from the Government of Russian Federation № 14.Z50.31.0027.

SUMMARY

In this presentation, Professor Grigorenko will focus on the current state of knowledge regarding major threats to the development of children growing up without their biological parents in different environments, namely different types of replacement families and institutions. Professor Grigorenko will provide an overview of the literature and particularly highlight aspects that are directly related to the research conducted by her Laboratory at SPbGU.

Professor Grigorenko will briefly outline the results of the first major adoption outcome study, How Foster Children Turn Out (1924), and milestone the subsequent work with regard to these early findings. Specifically, Professor Grigorenko will first discuss the types of care used around the world to support children growing without their biological families and, second, will focus on types of replacement families and other arrangements available to such children, particularly in the Russian Federation. Professor Grigorenko will provide an overview of the literature with regard to the major dimensions of child development, specifically, the child’s physical and neurological maturation, cognitive (including language) and social-emotional development, and, when available, longitudinal results and life-long outcomes such as academic and vocational achievement and physical and mental health.

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SCIENTIFIC ORGANIZATION
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Intrathoracic organs and tissues biological scaffolds creation in rat and nonhuman primate models

ABSTRACT

Regenerative medicine is a prospective scinetific direction allowing creation of artificial organs and tissues for replacement and restoration of native ones in case of their failure or damage under various pathological conditions. We believe that undernoted protocols of heart, lungs, diaphragm and esophagus matrices obtainment which were structurally and mechanically similar to native organs open the door to creation of clinically functional, fully tissue-engineered intrathoracic organs and tissue replacement in the near future.

KEYWORDS

Regenerative medicine, tissue engineering, decellularization, intrathoracic organs and tissues, scaffolds, bioreactor.

ACKNOWLEDGEMENTS

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SUMMARY

Tissue engineering as a part of the regenerative medicine is an interdisciplinary field, which applies principles of cell transplantation, materials science and engineering to develop biological substitutes that establish or restore physiological function. The one of three main principles of tissue engineering is use of a scaffold, i.e. a three-dimensional structure for cells to adhere to and grow on which can be either natural or artificially derived. Perfect biomaterial scaffolds for intrathoracic organs and tissue grafts should be non-toxic, resistant to infection, durable, elastic, biodegradable and supporting in vitro adhesion, growth and function of several cell types. In vivo acellular matrices should act as a template allowing the ingrowth of host cells and remodeling into a living tissue. Biomaterials should not: provide inflammatory reaction or rejection, allergy or sensitization, shrink in the healing process, be carcinogenic or initiate local complications. For biologically derived scaffold creation we used decellularization of donor organs. Decellularization involves use of physical or chemical means to eliminate immunogenic cells from an organ or tissue while preserving a native ultrastructure and composition of the extracellular matrix (ECM), which maintains biomechanical properties of the organ. An optimal decellularization method varies depending on the tissue/organ. For intrathoracic organs and tissues (heart, lungs, diaphragm, esophagus) decellularization in rat and nonhuman primate models a detergent-enzymatic method (DEM) was used. We applied a modified protocol with reduced detergent and enzymes exposure time and sequence: [Aqua MilliQ, Deoxycholate 4% (Sigma, Sweden), Triton-X 100 (Sigma, Sweden), PBS, DNAse I, 2000ku in 200ml PBS (Invitrogen, Sweden), EDTA, 800 um in 200 MilliQ (Sigma, Sweden)]. Absence of nuclei and other cell elements was demonstrated in decellularized organs. Moreover, the reciprocal orientation of fibers in scaffold walls resembled that of the control (i. e. native organ), and there also were no signs of collagen and elastin degradation. Architectonics of intrafibrous connective tissue remained intact and preserved adventitia of small vessels. Nuclear structures fluoresced intensively in native organs, while in decellularized organs no fluorescence was observed. In vitro studies revealed that 24 hours was necessary for complete removal of cellular part of tissue, including elimination of specific tissue protein tropomyosin and MHC class I, MHC class II, von Willebrand factor. We determined that these protocols have a minimal negative impact on extracellular matrix composition, ultrastructure and biocompatibility properties. Our suggestion was confirmed by undamaged histo-architecture and ultrastructure

(SEM) of extracellular matrix without fragmentation or structure loss. Moreover, we observed presence of extracellular proteins such as collagen I, collagen IV, laminin, fibronectin, elastin. Lack of immunogenicity was also confirmed by DNA quantification of decellularized matrices. Moreover, decellularized matrices preserved important biomechanical properties. Measuring of mechanical properties demonstrated that both native and decellularized organs possess almost the same properties. Our data obtained in vitro from MTT assay, Live/Dead assay suggested that the seeded graft contained attached cells that were viable and proliferating on surfaces. It could be demonstrated that matrix degradation products did not exert any toxic effect on cell viability.

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What drove the evolution of humans and hominids: the case study of core promoters evolution

SCIENTIFIC ORGANIZATION

Center of Brain Neurobiology and Neurogenetics, Institute of Cytology and Genetics SB RAS

ABSTRACT

Modern humans possess at least one feature that makes them be strongly different from anthropoids (chimpanzee and gorilla): being eurybiontic. To find evidence of selection for widening the norm of reaction of the genotype in human lineage, we have focused on the structural and functional evolution of the core promoters of human genes. It has been demonstrated that the spectrum of epigenetic possibilities for regulation in the core promoters of genes accumulated during the evolution of human lineage. In the ape lineages, the reverse is true: changes that narrow this spectra prevail.

KEYWORDS

Wide norm of reaction of the genotype, core promoters evolution, human, hominids.

ACKNOWLEDGEMENTS

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SUMMARY

Whole-genome comparisons of protein-coding sequences between humans and chimpanzees or gorilla suggest that they differ by 1 2% only, which is in sharp contrast with the significant morphological and ecological differences. There are sets of functionally-related genes, which are most strongly driven by adaptive evolution. In all three species, the primary evolving entities were spermatogenesis, receptors, the immune system, genes for signal transduction (for example, G-proteins) and embryogenesis regulation [1-5]. It was anticipated that the elevated rate of the evolution of certain brain genes observed in the human lineage would be species-specific. However, to date a very few genes have been found showing prominent brain-specific expression along with a signature of an adaptive evolution of protein-coding sequences in humans, but not in other anthropoids [1-5]. Missense- or loss-of-function mutations in genes showing accelerated evolution in human lineage may lead to severe pathologies and can be deleterious in human and animal populations [3]. It is conceivable that the selection acting on compensatory genetic variants interfering with deleterious mutations may also contribute to the process of adaptive evolution. Modern humans possess at least one feature that makes them be strongly different from anthropoids (chimpanzee and gorilla): the broad tolerances to the environment or, as Th. Dobzhansky spoke – “man is genetically specialized to be unspecialized” [6]. As a result, humans can live in a broad spectrum of habitats and landscapes, spreading across the continents [7-9]. This broad tolerance to the environment is associated with a widening norm-of-reaction [10] of the genotype [11]. Consequently, the sought-for hominoid-specific vector of selection may have been directed at widening the norm-of-reaction, that is, being associated not so much with the reduced or increased level of expression of the specific genes as with the enhanced regulatory plasticity of the genes

or ability to vary the gene expression level within a broad range. To our knowledge no search for evidence of such selection using whole-genome data has been performed as yet.

In this study, we focused on the structural and functional evolution of the core promoters of human genes, especially of those expressed in the brain prefrontal cortex. In 2011, a map with TATA-box locations for 17181 human genes was reported [12]. At that time, the map was exclusively based on Cap-analysis gene expression (CAGE) data counting capped 5' ends of transcript sequences. At present, the location of a gene promoter is considered to be clearly determined if more than one independent experimental approaches identifies the same position [13, 14]. In this study, the positions of promoters were inferred from two independent sources of experimental information: 1) CAGE data obtained from a large number of tissue-specific experiments, and 2) ChIP-seq data revealing the presence of transcriptionally active promoters in certain genomic regions marked by trimethylated histones H3K4 (H3K4me3), a chromatin protein associated with transcriptional start sites (TSS). According to modern views, transcription does not proceed continuously, but by jerks called "transcriptional bursts", the magnitude of which "is a promoter-specific property that is relatively robust to sequence mutations but is strongly dependent on the interaction between the TATA box and promoter nucleosomes" [15], which, in turn, is dependent on the abundance of CG dinucleotides in the promoter [16]. Moreover, there are a plenty of papers arguing whether increasing CpG sites (DNA regions enriched with CG dinucleotides) in a promoter can increase the range of transcriptional levels [17, 18]. Considering this view, we have performed an analysis of the evolution of three features of the upstream region of core promoter [600; -1]: (1) appearance or disappearance of CG dinucleotides, (2) predicted nucleosomal packing levels (nucleosome/DNA affinity), and (3) predicted affinity for TATA-binding protein (TBP/DNA affinity).

As a result, we demonstrated that the trend to increased spectrum regulatory capacities for the core promoters of genes accumulated during the evolution of two ancestral lineages preceding the divergences the ancestor of all hominids (humans, chimpanzee and gorilla) and the divergence of chimpanzee and humans was continued in the evolution of human lineage. In the anthropoid lineages (chimpanzee, gorilla and orangutan), the reverse is true: changes in promoters that narrow this spectrum prevail. This implies that, first, the origin of *Homo sapiens* is associated with a selection for widening the norm-of-reaction of gene expression regulation. Second, by contrast, the origins of the three ape species (especially gorilla and chimpanzee) are associated with a species-specific selection for narrowing the norm-of-reaction of gene expression regulation. Third, the selective trend towards widening the norm-of-reaction of gene regulation in the hominids is quite ancient – at least more ancient than the chimpanzee/humans split event occurring 5-6 million years ago.

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Solid-binding peptide linker for targeted nanocomposites

SCIENTIFIC ORGANIZATION

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ABSTRACT

A facile strategy was developed to construct targeted nanocomposites based on silica-coated upconversion nanoparticles (UCNP-SiO2) and bioconjugation to tumor-targeting antibodies through a bifunctional fusion protein (LPG) consisting of a solid-binding peptide linker genetically fused to Streptococcus Protein G'. The prepared nanocomposites were showed to specifically target tumor cells overexpressing cancer-characteristic antigens.

KEYWORDS

Solid-binding peptides, upconversion nanoparticles, targeted imaging.

ACKNOWLEDGEMENTS

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SUMMARY

Targeted constructs for the tumours diagnosis and therapy based on photoluminescent nanoparticles are among the most rapidly developing areas of present-day biomedicine. These particles possess unique photophysical properties and their surface allows to use them as a platform for diverse targeting/therapeutic

biomolecules. Upconversion nanoparticles (UCNPs) are one of the most perspective kinds of photoluminescent substances. The UNCPs are capable of efficient conversion of near-infrared (NIR) excitation at the wavelength of 980 nm into the shorter-wavelength infrared and visible spectral range emission. UNCPs are also inherent high spatial-temporal resolution in bioimaging [1], low cytotoxicity and long lifetimes [2]. Their near-infrared excitation band falls into the “biological tissue transparency window”, which allows the excitation light to penetrate deep into the biological tissue [3].

To minimize the side effects of tumor visualization and treatment UCNP nanocomposites are required to bioconjugate to active tumor-targeting moieties such as peptides [4] and antibodies [5]. The conventional bioconjugation techniques may reduce the functional activity of the targeting and lead to the particle aggregation. Therefore, new strategies of assembling UCNPs and targeting moieties while maintaining their functionality and selectivity, are highly desirable.

We have developed a facile strategy to construct nanocomposites functionalized for cancer targeting, based on coating of the UCNP with a silica layer and bioconjugation to antibodies (Ab) through a bifunctional fusion protein (Linker-Protein G, LPG). LPG consist of a solid-binding peptide linker (L) genetically fused to *Streptococcus* Protein G’ (PG). Solid binding peptides are short amino acid sequences that selectively bind to their corresponding solid surfaces with high affinity through a combination of multiple non-covalent interactions (e.g. van der Waals forces, electrostatic, hydrophobic, and π effects) [6]. The solid binding peptide linker used here (with a sequence of $(VKTQATSREEPPRLPSKHRPG)_4VKTQTAS$) is capable of mediating the specific binding of the LPG to silica-coated nanoparticles across a wide pH range (5-9) [7]. The Linker domain of LPG exhibits high binding affinity towards silica surface, and the IgG-binding protein binds to the Fc fragment of IgG antibodies, thereby ensuring the functional display of the conjugated antibodies. Thus, LPG mediates the functionalization of silica-coated UCNPs (UCNP-SiO_2) with cancer cell antibodies allowing for specific target recognition and delivery.

The core UCNPs ($NaYF_4$:Yb,Er) were synthesized using a solvothermal decomposition method. An inert shell of $NaGdF_4$ was further deposited onto the core UCNPs. The core-shell UCNPs ($NaYF_4$:Yb,Er/$NaGdF_4$) retained their morphology and dispersion, and had an average diameter of 31 ± 1 nm. Compared to the core UCNPs, the core-shell UCNPs exhibited 1,7-fold enhanced upconversion photoluminescence under continuous-wave 980-nm excitation. A thin layer of silica (SiO2) was coated onto the core-shell UCNPs using a water-in-oil microemulsion method to improve aqueous solubility and stability of UCNPs in physiological environments. The resulting UCNP-SiO_2 particles were spherical in shape, with a mean diameter of 43 ± 2 nm.

UCNP-SiO_2 were bioconjugated to LPG and monoclonal antibody for epithelial cell adhesion molecules (EpCAM, also known as CD326) via simple mixing and washing steps. EpCAM is a transmembrane glycoprotein that is expressed at low levels in normal epithelia but overexpressed in epithelial cancers (i.e. carcinomas), and is a recognized target for immunotherapy [8].

The *in vitro* binding ability and specificity of the functionalized UCNP-SiO_2-LPG-Ab nanocomposites were examined using HT-29, an EpCAM-overexpressing human colon adenocarcinoma cell line, and BV2, an EpCAM-negative murine microglia cell line. Each cell line was incubated with 25 μg/mL nanoparticles for 1 h and washed five times before fluorescence imaging. The UCNP nanocomposites selectively labeled the membrane of the EpCAM-positive HT-29 cells. In contrast, negligible UCNP nanocomposites were observed with the EpCAM-negative BV2 cells.

These results confirm that the LPG-mediated bioconjugation approach allows the anti-EpCAM to maintain good targeting capability when conjugated onto the UCNP nanocomposites, and LPG can be successfully used for attachment of targeting antibodies onto silica-coated UCNPs.

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Individual variability of brain neuronal chromatin: implication to schizophrenia

SCIENTIFIC ORGANIZATION

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ABSTRACT

Schizophrenia is a highly heritable neuropsychiatric disorder; but genetic and non-genetic factors for development of this disease are largely unknown. We have analyzed whole-genome epigenetic profiles of open chromatin loci for a cohort of schizophrenia and control individuals, focusing specifically on cortical neurons. The analysis of these profiles provides a unique insight into gene promoter activities and its dysregulation in schizophrenia pathology. We have highlighted a number of novel and known genomic loci, which potentially contribute to the disease development.

KEYWORDS

Schizophrenia, epigenetics, chromatin, H3K4me3, brain, neuron.

ACKNOWLEDGEMENTS

This work was partly supported by the Government of the Russian Federation (grant 14.B25.31.0033).

SUMMARY

Schizophrenia is a devastating neuropsychiatric disorder affecting approximately 1% of the global population. The predisposition factors for developing schizophrenia are largely unknown, yet it is highly heritable, suggesting that genetics play a significant role. However, to date genetic studies did not completely uncover the genetic roots of schizophrenia. Non-genetic factors are also mostly unknown; and some of them can may be epigenetic modifications. Recent technology advances now allow quantifying these modifications; specifically chromatin modifications can be measured by chromatin immunoprecipitation followed by sequencing (ChIP-seq). We took advantage of this method to evaluate the transcriptional activity in brain neurons of individuals diagnosed with schizophrenia to identify genomic loci and genes, which are responsible for disease development.

In this study, we profiled chromatin modifications (specifically, H3K4me3, a marker of active transcription) in brain neurons of schizophrenic and control individuals by ChIP-seq and identified a number of genomic loci that differ in norm and pathology; they include known schizophrenia genetic risk loci and novel, previously not reported, regions. The findings of this study provide an insight into modifications of transcription activity specifically in brain neurons in schizophrenia; it also highlights a number of genes and pathways potentially involved in schizophrenia pathogenesis.

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Seasonality of influenza. The Role of environmental factors and supersaturation in the lungs in airborne transmission of respiratory infections

SUMMARY

Airborne transmission refers to infectious diseases that spread via bioaerosols (droplets and particles below 5 μm) containing viruses or bacteria and can lead to global pandemics.

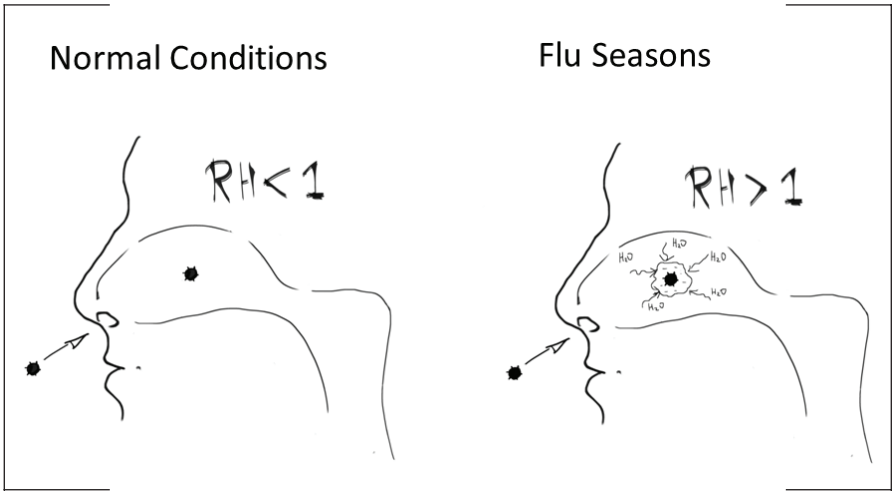
The latest researches shown the infected people when breathing generate the infectious aerosols with particles below 1 μm. The airborne transmission of these particles is effective but the deposition of submicron particles in the respiratory tract (RT) has very low probability.

Here we investigated the processes in RT when breathing cool/cold air and its role in the delivery of viruses and bacteria of submicron sizes in RT.

On the basis of systematic review and numerical estimation we have originally shown: *Breathing cool/cold air leads to the oversaturation of air in RT; the air oversaturation leads to the intensive condensational growth(CG) of inhaled viruses or bacteria in RT; CG leads to the intensive deposition of viruses or bacteria in RT.*

The estimation shown that for conditions of breathing cold air of T [-15..+15]°C and Relatively Humidity (RH) of [30..60]% the concentration of liquid water in the mixed air in RT (C_{Liq}) is [0·2..12·1]g/kg. Under these conditions the growth of inhaled particles by condensation in RT is significant.

Under normal conditions of inhaled air (T>20°C; RH=60%) there is no transition in oversaturated condition in RT (CG is insignificant and probability of virus deposition on epithelium of RT is low).



But with an increase in RH of inhaled air the oversaturation in RT occurs even at warm temperature of inhaled air. For inhaled air of T=20°C, RH>70% - C_{Liq}<2·4g/kg and for T=25°C; RH>90% - C_{Liq}<1·2g/kg.

These results correspond to seasonality of influenza and respiratory infections in temperate and tropical climates and indicate the high probability of virus deposition on epithelium of RT.

It may be the key to '*the age-old epidemiologic mystery of influenza seasonality in the different climatic conditions'*.

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SCIENTIFIC ORGANIZATION

Kazan Federal University

GABAergic functions in the developing neuronal networks

KEYWORDS

GABA, development, cerebral cortex, network activity, patch-clamp.

SUMMARY

During development, GABA, which is the main inhibitory neurotransmitter in cerebral cortex, exerts paradoxical excitatory actions on the immature neurons. Excitatory actions of GABA during development are due to the elevated intracellular chloride concentration and thus depolarizing direction of currents through GABA(A) ion channels. However, the roles of GABAergic mechanisms in the operation of immature neuronal networks remain poorly understood. Recent studies have provided important insights into the understanding of how GABA controls activity in the developing cortical networks. Firstly, using gramicidin perforated patch recordings from CA3 pyramidal cells we have shown that during generation of the recurrent network bursts in the neonatal rat hippocampal slices in vitro (so-called Giant Depolarizing Potentials), GABA transiently switches its action from depolarizing/excitatory to hyperpolarizing/inhibitory. These dynamic changes in the GABAergic actions on principal neurons enable GABA not only to initiate network bursts, but also to inhibit neuronal network at the peak of the network excitation. Moreover, using optogenetic approach in the mice expressing photoactivated channelrhodopsin in GABAergic interneurons, we have shown that in the neonatal cortex in vivo GABA reduces the frequency of glutamatergic postsynaptic currents and thus exerts mainly inhibitory actions in the developing cortical networks. These findings indicate that GABAergic functions are more complex than simplistic view on GABA as purely excitatory neurotransmitter despite of its depolarizing actions in the developing brain. The complexity in the actions of depolarizing GABA at the network level may be important not only during development but also in a number of pathological states including epilepsy, trauma and pain, where depolarizing shifts in the GABA actions may occur.

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SCIENTIFIC ORGANIZATION

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Protein corona formation on polymer-coated nanoparticles

ABSTRACT

Biofuncational nanomaterials are ushered into the era of theranostics offering new possibilities for diagnosis and treatment. Their surface grafted with functional biomolecules is swiftly remodelled as soon as they enter biological fluids, such as blood serum – the process termed “protein corona”. We report on investigation of how the protein corona is formed on polymer-coated upconversion nanoparticles (UCNP) by using transmission electron microscopy, dynamic light scattering, protein assaying and fluorescence correlation spectroscopy.

KEYWORDS

Upconversion nanoparticles, protein corona, theranostics.

ACKNOWLEDGEMENTS

This work was supported by grant No. 14.Z50.31.0022.

SUMMARY

Development of new approaches for the diagnosis and therapy of tumours (taken together, termed theranostics) - one of the most dynamic areas of biomedicine,

where new nanomaterials afford new opportunities. The nanomaterial merits include: programmability of their physical and chemical properties; abundance of reactive functional groups on the surface; large effective surface area; optimum size, which determines preferential accumulation of nanoparticles (NPs) in tumour tissue[1]. Understanding of how engineered nanomaterials interacting with biological systems and environment is presently a most exciting research topic at the interface between nanotechnology and the life sciences.[2-4] It is increasingly being accepted that NPs encountering biological medium are swiftly coated by a biomolecular adsorption layer, the so-called "protein corona".[5,6] Consequently, the molecular machinery of a living cell or organism will – at least initially – interact with the corona rather than the bare NP, making it a key determinant of the biological response of NP exposure. Indeed, studies have reported that protein adsorption onto NPs affects their cellular uptake efficiency, controls the internalisation mechanism,[7] and modulates pathobiological effects.[8] Therefore, a profound knowledge of the protein corona, including its composition, structure, dynamics and thermodynamics, is of fundamental importance for the safe and well controlled application of NPs.

As a model NP, we choose upconversion nanoparticles (UCNPs) allowing background-free optical imaging[9], which make them attractive for applications in life sciences[10]. UCNPs in the form of hexagonal crystallites $NaYF_4$ doped with Yb^{3+} and Er^{3+} or Tm^{3+} were synthesised in the size range of 20 – 30 nm by a modified solvothermal method[11] [see Figure 1 (left panel)]. UCNPs were coated with three types of polymers: positively charged polyethylenimine (PEI), negatively-charged polyacrylic acid (PAA) and neutral-negative polyethylene glycol (PEG), which is regarded as excellent dispersant. Although incubation with mono-component plasma protein solution (e.g. bovine serum albumin - BSA) displayed well-studied formation of a monolayer of BSA on the surface of UCNP [Figure 1 (middle panel)], its incubation in fetal bovine serum (FBS) displayed profound protein corona formation, followed by some degree of aggregation [Figure 1 (right panel)].

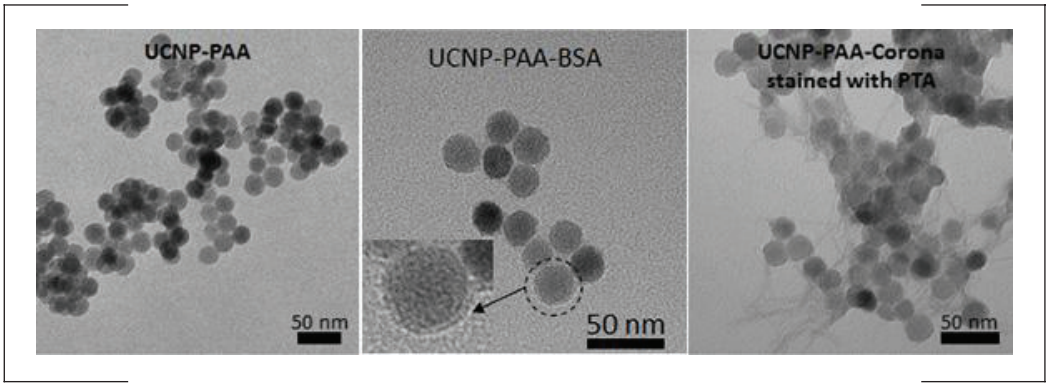

Figure 1. TEM images of UCNPs-PAA, shown in left panel. Middle panel, TEM image of UCNP-PAA incubation with BSA, with an arrow showing a monolayer of BSA. Right panel, TEM image of UCNP-PAA incubated in cell culture medium at 37 °C for 24 h stained with 2% phosphotungstic acid (PTA).

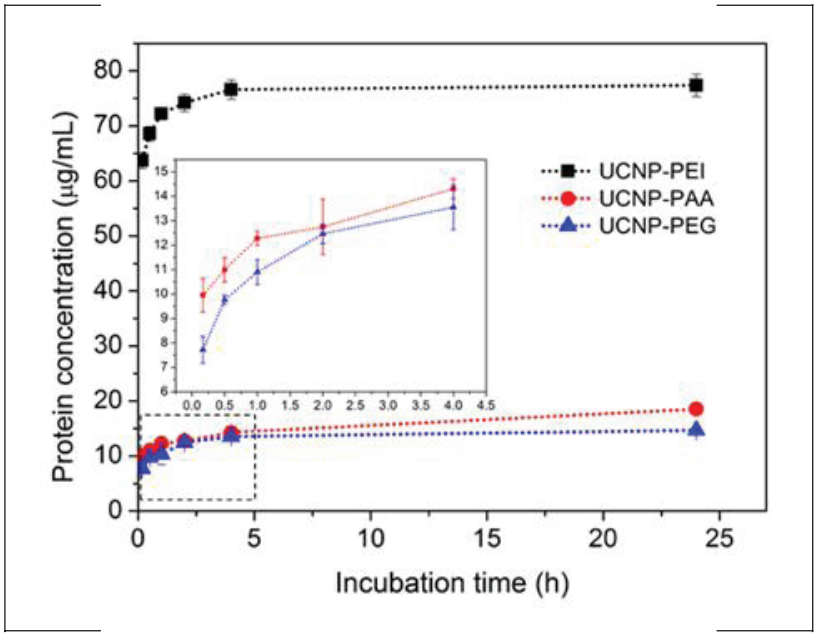

Figure 2. Temporal development of protein corona on UCNP-PEI, UCNP-PAA, and UCNP-PEG at 10 min, 30 min, 1 h, 2 h, 4 h and 24 h, measured by Micro BCA assay. Protein corona was formed by incubating 1 mg of UCNP in 1 mL of cell culture medium (DMEM+10% FBS) at 37 °C for different time points. After removal of soft corona via three wash steps, the hard protein corona mass was estimated by colometric BCA assay using the BSA standard curve. Abbreviations: BCA, bicinchoninic acid.

Our protein assaying study corroborated the TEM observation, as shown in Figure 2. It shows profound effect of the UCNP-polymer surface charge. In particular, UCNP-PEI acquired almost ten-fold of protein content as compared to that of UCNP-PEG and –PAA. Figure 2 (inset) also shows that the protein binding occured within minutes, which is in agrement with the literature[12].

The zeta-potential measurement showed the surface charge became more negative. The protein corona of FBS origin enhanced the surface binding and internalisation of all types of UCNPs.

We will report on our results on the protein corona formation by means of fluorescence correlation spectroscopy, which provides a very valuable *in situ* measurements means.

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SCIENTIFIC ORGANIZATION

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Portable bioluminescent laboratory for ecological and medical toxicity monitoring

ABSTRACT

Laboratory consists of a bioluminometer «LumiShot», a multicomponent immobilized reagent «Enzymolum» and a set of toxicity bioassays for medical, environmental and industrial application such as evaluation of water, air and soil pollution, assessment of materials toxicity, the of endotoxicosis and stress degree etc. A new educational practical courses are suggested. The laboratory allows for fast (3-5min) detection of a wide range of the chemical and biological toxic compounds. The advantages of enzymatic assays are high sensitivity, validity, simplicity of methods.

KEYWORDS

Bioluminescence, bioluminometer, practical course, immobilized reagent, portable laboratory.

ACKNOWLEDGEMENTS

The research was funded by project «Bioluminescent biotechnology» (agreement № 11.G34.31.0058).

SUMMARY

Laboratory consists of a bioluminometer “LumiShot”, multicomponent immobilized reagent “Enzymolum” and set of toxicity bioassays for medical, environmental, and industrial application such as evaluation of water, air and soil pollution, assessment of the toxicity of nanomaterials, medical materials and food additives, the degree of endotoxicosis, the effect of physical load on sportsmen, and in new practical courses for higher educational institutions and schools. The multi-component reagent “Enzymolum” contains the bacterial luciferase, NADH:FMN-oxidoreductase and their substrates, co-immobilized in starch or gelatin gel. Laboratory immediately signals chemical-biological hazards and allows us to detect a wide range of toxic substances. The advantages of enzymatic assays are their rapidity (the time of analysis does not exceed 3-5 minutes), high sensitivity and validity, simple measuring procedure, stability and safety of reagents.

The multicomponent immobilized reagent “Enzymolum” is the main part of laboratory [1]. In this study, we propose a new approach to design enzymatic reagent kits based on selecting the conditions for co-immobilization of various components of enzyme systems in natural gels with their subsequent drying. The method for creating multicomponent enzyme preparations is illustrated by the example of the reagents for bioluminescent analysis based on coupled enzyme system of luminous bacteria NAD(P)H:FMN- oxidoreductase and luciferase (Red + Luc). In our study, reagent components (NAD(P)H:FMN-oxidoreductase and luciferase and their substrates NADH and myristic aldehyde) were immobilized in starch or gelatin gels. Thus obtained multicomponent immobilized reagent contains all the components required for one measurement except FMN which is added as a solution to start the reaction of light emission. The reagent represented a dried disk 6-7 mm in diameter, whose dry weight was 1.5 mg. By varying the composition of the multicomponent reagent and the microenvironment of enzymes in the reagent, it is possible to obtain a family of immobilized enzyme preparations whose characteristics vary depending on the analytical task to be solved. In the study we varied the ratio of components in the immobilized reagent; the chemical nature of the gelling agents (starch or gelatin) and their concentration; the concentration of agents stabilizing the enzyme activity and conditions of the immobilized reagent drying. We analyzed such characteristics of immobilized reagents as activity estimated by the maximum of the light intensity (I_{max}), time when the coupled enzyme system reached the luminescence maximum (T_{max}), sensitivity to toxic compounds and stability during long-term storage. We found that a decrease in the content of enzymes or substrates in the reagent increased its sensitivity to toxic compounds. The reagent obtained by co-immobilization of the enzymes and substrates in the gelatin gel had a higher activity and stability during storage than those based on the starch gel, but it showed a lower sensitivity to toxic substances. An increase in the concentration of gelatin significantly increased the T_{max} value, which, in turn, increased the duration of analysis. The best combination of high activity with stability during storage was reached by the addition of 100 μM DTT to the reagent. Multicomponent immobilized reagents (variants of “dry chemistry” reagents) can be used not only for routine assays but also as modules in biological enzymatic biosensors. Moreover, the proposed approach can be widely used for preparing reagents for not only bioluminescent but also other types of enzymatic assays.

This review describes the principle and applications of bioluminescent enzymatic toxicity assays. The new approach to develop the bioluminescent enzymatic biosensors, toxicity bioassays and reagents has been described. To solve the problem of how to detect, identify, and measure the contents of the numerous chemical compounds in environmental monitoring, food product monitoring, and medical diagnostics, the bioluminescent enzymatic toxicity assays were, wherein the bacterial coupled enzyme system NAD(P)H:FMN-oxidoreductase-luciferase substitutes for living organisms. Historically, the application of bacterial luminescence in toxicology began with the usage of luminous bacteria for ecological monitoring and they are still widely used. These methods made it possible to determine environmental pollution by comparing the light emission intensity of luminous bacteria in the control and in the analyzed samples. As opposed to other test objects such as paramecia, algae, crustaceans, and so on, the bioluminescent assay was faster (the time of analysis didn’t exceed 30 min). However, as with other living organisms, the essential disadvantage of this method was low accuracy of measurement caused by the “petulance” of living luminous bacteria: failure to maintain the stable state of bacterial culture during measurements and storage. The bacteria reacted to the appearance of toxic substances either by decreasing or by increasing the luminous intensity, which often led to ambiguous interpretation of results. That’s why only qualified staff could work with bacteria. Because of these shortcomings

an assay based on luminous bacteria didn't show very good results in ecological laboratories. To overcome those difficulties it was suggested to use enzymes of luminous bacteria in soluble and immobilized forms. Since 1990, a new trend in bioluminescent toxicity analysis named bioluminescent enzymatic toxicity assay has been developed [2]. At present, it is actively used in ecology, medicine, agriculture, and other areas [3, 4].

The main principle of the bioluminescent toxicity enzymatic assays is inhibition of couple enzyme system: Red + Luc by the toxic components of analyzed samples. The principles of bioluminescent enzymatic toxicity assay were successfully used for the analysis of aquatic environments as well as air and soil pollutions. With bioluminescent enzymatic toxicity assay there is possibility to solve a problem of complex evaluation of environmental toxicity. It is well-known that to estimate environmental toxicity it is necessary to use the battery of bioassays. Usually they represent different levels of life organizing such us cells, organs, organisms and ecosystems. Due to the coupling with bacterial luciferase, it is possible to design new enzymatic assays in toxicology and combine them into a set to provide the toxicity control at the enzymatic level. The set includes enzymes of different classes, or key enzymes of metabolic processes in living organisms. The bacterial luciferase may be the terminal enzyme in coupling chains for more than 100 enzymes including such as lactate dehydrogenase, trypsin, glucose-6-phosphate dehydrogenase, and others, making it possible to measure the enzyme activities according to the light emission intensity. To develop the set of bioluminescent enzymatic toxicity assays different enzyme interaction mechanisms were suggested. As an example to estimate toxicity of water samples two enzymes were chosen: alcohol dehydrogenase (ADH) and trypsin, because they belong to different classes (oxidoreductases and hydrolases), and secondly, because they interact differently with bacterial luciferase, providing different sensitivity to the toxic substances. The effect of toxic substances on the activities of the triple enzyme system with ADH and trypsin were measured using the bioluminescence decay constant. The set of bioluminescent enzymatic toxicity assays was used for monitoring natural and laboratory aquatic ecosystems and for studying the seasonal dynamics of zooplankton non consumptive mortality.

Examples of application the set for toxicity analysis of pesticides and sanitary assessment of natural polymers polyhydroxyalkanoates are given too. Bioluminescent enzymatic assays are used in other sectors, such as agriculture and food industry. The first example is evaluation of wheat grain infection with *Fusarium*. Mycotoxins of fungi of the genus *Fusarium* in feeding causes poisoning and even death of animals. International standards for grain quality and medical and biological requirements for food quality require that grain contamination with *Fusarium* should be controlled at the stages of crop harvesting, purchase, and processing. To develop rapid analysis of wheat grain infection with *Fusarium* the effects of their mycotoxins on the coupled enzyme system were studied at first and the strong inhibition of enzymatic activity was observed. The sensitivity of the coupled enzyme system Red + Luc to mycotoxins decreased in the following order: zearalenone, deoxynivalenol, toxin T-2, and diacetoxiscripenol. Further, in study it has been showed that the efficiency of Red + Luc activity inhibition by wheat extracts depended on the severity of grain infection with *Fusarium*. Moreover, the inhibition was caused not only by mycotoxins but also by other metabolites of *Fusarium*, which were accumulated in infected grain. The inhibition of bioluminescence depended on the geographical origin and growth conditions of the grain. These differences were able to minimize due to the method of sample preparation. Another example is assessment of food additives safety. The sodium benzoate (E 211), potassium sorbate (E 202) and sorbic acid (E 200) were tested. The effects of nanomaterials such as Ag, Cu, Cu_2O which have the prospect of introduction to the food technology also were identified. The loss of light emission intensity of the coupled enzyme system Red + Luc in the presence of food additives was estimated. Also the toxic effects of additives on the bioluminescence of the three triple enzyme systems Red + Luc + trypsin, Red + Luc + ADH and Red + Luc + LDH (lactate dehydrogenase) were analyzed. Results were compared to the well-known tests based on survival and chemotaxis ciliates *Paramecium caudatum*, germinating of shoots and roots of cress "Cudriavyy", survival of *Daphnia magna*, changes in the level of chlorophyll fluorescence of algae *Scenedesmus spp.* and foaming by the yeast *Saccharomyces cerevisiae*. The effects of the food additives on organisms were evaluated using parameters EC_{50} or LD_{50}. The coupled enzyme system Red + Luc and triple enzyme system with LDH showed a great sensitivity to the analyzed food preservatives. Values of EC_{50} were equal 0.03, 0.14, 0.008 and 0.66, 0.13, 0.07 mM for sodium benzoate, potassium sorbate and sorbic acid, respectively. The values of EC_{50} estimated by enzymatic

tests were over two times less than that for the biological tests mentioned above. The maximum decrease in the relative activity of trypsin and ADH assays did not exceed 45 % in the studied range of preservatives concentration. It was shown that both copper and copper oxide (I) nanoparticles had a strong inhibitory effect on Red + Luc system. Values of EC_{50} were equal 4 μM and 1.5 μM for copper nanoparticles and Cu_2O, respectively. Value of EC_{50} for silver nanoparticles was 0.18 mM. The bioluminescent enzymatic toxicity assay indicated the negative effect of food additives in the much lower concentrations than its actual maximum content in food products. There is a problem which is extremely topical both for agriculture and food industry. It is pesticides. Pesticides vary in their toxicity mechanism and character, e.g. they can be carcinogenic or mutagenic, or they can affect the respiratory, endocrine, immune or nervous systems. There are two different types of pesticides: organophosphates and pyrethroids. Organophosphorous substances are complex esters of phosphoric acid and their toxic effect is accounted for by their ability to inhibit acetyl cholinesterase, the key enzyme in synaptic transmission in nerves. Pyrethroid insecticides, synthetic analogues of natural pyrethrins, act through intestinal contact, thereby affecting the nervous and the immune systems. In our study the set of bioluminescent enzymatic toxicity assays was applied to analyze toxicity of organophosphorous and pyrethroid pesticides. The sensitivities of the bioluminescence assays were close to those determined by other biological assays or even higher. The triple enzyme systems with ADH and trypsin have been shown to be more sensitive to organophosphorous compounds (0.13–11 $mg \cdot L^{-1}$). Sensitivities of the triple enzyme systems to pyrethroid pesticides were similar to those of *in vivo* assay based on luminous bacteria (0.9–5 $mg \cdot L^{-1}$).

The bioluminescent enzymatic toxicity assay is also very promising for medical research, for example, for evaluating the gravity of endotoxicosis during treatment in surgery and therapy. It is based on the fact that the effect of donor's blood serum on enzymatic activity differed markedly from that of the patients': blood serum of a patient inhibits bioluminescence less than that of donor. Two modifications of the assay using luciferase and coupled enzyme system Red + Luc have been developed. Comparative analysis of application efficiency for luciferase index LI and other laboratory parameters to assess the severity of patients with peritonitis have been made. Bioluminescent enzymatic toxicity assay allows to estimate the severity of a patient's condition as satisfactory, of middle seriousness, severe and the critical one. It can be used also for disease course prediction, estimation of the efficiency of the used detoxification methods, and control of drainage procedure with semipermeable membranes. Most important is applying LI in prognostic plan as far as the long positive LI dynamics could indicate the need for change of treatment plan. It was reported that the assay can be used as a reliable criterion to monitor the course of disease for therapeutic patients with bronchitis, ulcerous disease or chronic colecystitis. The most important advantages of the proposed approach are the very short time interval between sample collection and results, high sensitivity, low traumatism, and simplicity.

A very interesting and promising trend in the development of bioluminescent enzymatic toxicity assay is the creation of rapid analysis for the assessment of human organism reaction to physical and mental stress. Analysis is made by comparing the light emission intensity of the coupled enzyme system Red + Luc in the presence of a person's saliva taken before and after a certain stress load. The main advantage of the assay is noninvasiveness, because human saliva is analyzed, which reflects the functional state of a person just as blood does.

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The role of PDLIM4/RIL gene in the development of breast cancer

SCIENTIFIC ORGANIZATION

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ABSTRACT

The aim of the research was to analyze mechanisms of PDLIM4 participation in the development of breast cancer. As a result of the work we examined the subcellular colocalization of Scribble with different isoforms of PDLIM4 and revealed differences between alternative transcripts of PDLIM4.

KEYWORDS

PDLIM4, breast cancer, Scribble.

ACKNOWLEDGEMENTS

The results of the project were achieved with support of the Ministry of Education and Science of the Russian Federation as a part of the agreement 14.607.21.0062 of the federal Special-Purpose Programme «Reseach and development in the high priority development fields scientific and technological complex of Russia for 2014 – 2020».

SUMMARY

PDLIM4 (PDZ and LIM domain protein 4) is an adaptor protein, encoded by the PDLIM4 gene. Epigenetic suppression of PDLIM4 is frequently associated with different types of cancer, particularly with breast cancer. The role of PDLIM4 in breast cancer development has not been sufficiently studied, so today there is no any theory, which could clearly explain correlation between changes in PDLIM4 expression and tumor progression. Previously, basing on our results, we had hypothesized a mechanism of Scribble-mediated participation of PDLIM4 in the development of breast cancer. According this theory RIL possibly interacts with Scribble - a membrane protein, which is involved in migration, proliferation and polarity of epithelial cells. The aim of the present research was to examine the subcellular colocalization of Scribble with different isoforms of PDLIM4, to verify the previously described hypothesis and reveal differences between alternative transcripts of PDLIM4.

At the first stage of our work we analyzed the expression of PDLIM4 in cells of different breast cancer cell lines. Among them we chose the cell cultures, which were characterized by expression of alternative transcripts of PDLIM4. The selected cells were used to examine differences in intracellular localization of alternative transcripts of PDLIM4 and compirison of this data with location of Scribble. The obtained data let us to estimate the relationships between Scribble and PDLIM4 and propose participation of single PDLIM4 isophorms in the process of Scribble-mediated epithelial-mesenchimal transition. Another outcome of our study was the finding, that alternative transcripts of PDLIM4 could be observed not only in cytoplasm, but into nucleus as well. The revealing of subnuclear localization of PDLIM4 let us to have another look on this protein, which had been previously described only as a cytoplasmic component.

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Computer modelling of the cardiac tissue layer formation

SCIENTIFIC ORGANIZATION

MIPT

ABSTRACT

Arrhythmias occur more frequently among older patients. However, all of the studies in ageing or diseased human heart are limited to the observation of the final histological pattern, whereas the dynamics of the preceding structural changes remains unclear. To fill this white space, we developed a large Potts model of the cardiac tissue layer formation, that describes precisely the cell shape of fibroblasts and cardiomyocytes, and model their segregation and formation of conduction pathways.

KEYWORDS

Large Potts model, cardiac tissue development, cardiac remodeling, cardiac arrhythmias.

ACKNOWLEDGEMENTS

We thank our colleagues — Alisa Podgurskaya, Hans Dierckx, Angelina Shutko, and many others — who contributed immeasurably to the insights in cellular spreading and cooperation.

SUMMARY

Cardiac arrhythmias, or even sudden cardiac death, may occur at any age, but the risks are increasing among older generation. It is known, that heart loses some of the active cells, which are replaced with the passive fibroblasts, the size of the heart slightly increases, the collagen is deposited between the bundles of cardiac myocytes, and, finally, the cardiomyocytes themselves change, as far as the expression of the ionic channels differs. However, it is poorly understood, which of these factors results in an elevated risk of arrhythmia. In fact, all of the studies of the ageing or diseased human heart are limited to the observation of the final histological pattern, whereas the dynamics of the preceding structural changes stay hidden from the clinical researchers. This white space may be filled with aid of computer modelling.

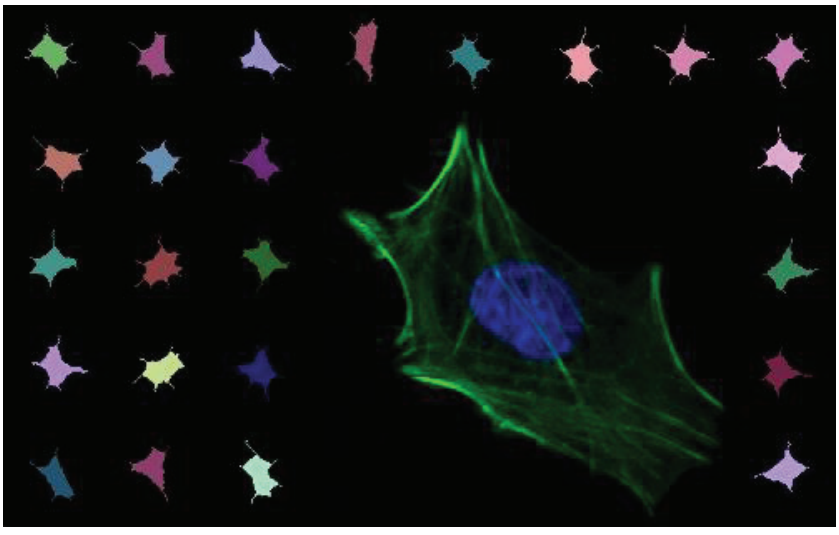

Figure 1. Cell spreading on an isotropic substrate. Single big cell shows an experimentally obtained image, where blue indicates nucleus and green — F-actin. Multiple coloured cells around it show the results of computer simulation with the same parameters of the large Potts model, but different random seeds.

The goal of our studies is to reveal the underlying mechanisms of cardiac tissue formation and to develop a mathematical model of this process. As a first step, we aimed to reproduce the growth of engineered cardiac monolayer on various substrates. First, we studied the spreading of the single cell of each type on the glass and on the nanofibrous net (see Fig. 1). Next, we observed cell-cell interaction and collective behaviour of the cells in monolayers: segregation of the cell types and formation of the conducting pathways. As a result, our model of tissue development takes into account two types of cells (cardiomyocytes and fibroblasts), their adhesion, elasticity, surface tension, and the parameters are adjusted to fit the experimental data for the monolayers of neonatal rat cardiac cell.

To simulate the development processes in cardiac monolayer, we utilised large cellular Potts models [1,2]. The morphogenesis of cells and tissues in this paradigm was already described for plant growth [3], angiogenesis [4], stem cell differentiation [5], *Dictyostelium discoideum* [6], epidermal formation [7], vascular system

development [8], etc. However, cardiac tissue was never studied with Potts models before. We explicitly introduced attachment sites and protrusion at the cell periphery, that was never done before. This approach allowed us to obtain a polygonal forms of the cells, which is characteristic for fibroblasts. Changing the ratio of elasticity and “spreading” forces, i.e. making the cell more rigid, turns cells into more cardiomyocyte-like shape and switches on polarization. Therefore, with this investigation we introduce a well-known tool from the field of developmental biology to serve as a basis for electrophisiological studies for a wide range of tissue growth conditions.

The ability to mimic tissue structure with engineered scaffolds coupled with *in silico* research provide us with a flexible tool for research in tissue development and analysis of the excitation propagation on the subcellular level. Our 2D mathematical model for the monolayer could be also extended to describe 3D tissue development, ageing and remodelling — the processes, that are impossible to observe in experiment.

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ADDITIONAL INFORMATION

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VDAC isoforms affect NAD(P)H-dependent redox processes and ROS generation in mouse embryonic fibroblasts

SCIENTIFIC ORGANIZATION

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ABSTRACT

The impact of VDAC isoforms on the redox processes in cells of mouse embryonic fibroblasts was studied. It was demonstrated that total NADH-ferricyanide reductase activity in VDAC1/3- cells was almost identical, while in VDAC2- cells increased in comparison with control. ROS production was increased several fold in the range wild type.

KEYWORDS

Mitochondria, VDAC isoforms, NAD(P)H-oxidoreductases, ROS, redox processes.

ACKNOWLEDGEMENTS

The study was supported by by grant from the Ministry of Education and Science of the Russian Federation, Agreement № 14.Z50.31.0028 and the Russian Foundation for Basic Research (project № 14-04-01664a).

SUMMARY

Mitochondrial voltage dependent anion channels (VDAC) play an important role in the metabolite exchange between cytosol and mitochondria in cell. For recent years at least five research groups reported that VDAC1 exhibits the NADH-oxidoreductase activity. Other works demonstrated that blocking of VDAC causes the overproduction of ROS. However, the mechanisms of these effects are unclear, since VDAC1 is neither classical oxidoreductase nor antioxidant enzyme. We studied the impact of VDAC1/3 and VDAC2 isoforms on the redox processes in cells of mouse embryonic fibroblasts (MEF). It was demonstrated that total NADH-ferricyanide reductase activity in VDAC1/3-lacking cells (MEF VDAC1/3-) was almost identical, while in VDAC2-lacking cells (MEF VDAC2-) significantly increased in comparison with control (MEF wt). The suppression of known outer membrane NADH oxidoreductase, cytochrome b5 reductase (Cyb5R3), caused statistically significant inhibition of ferricyanide reduction. In the same time, intracellular and mitochondrial ROS production increased several fold in the range MEFwt < MEFVDAC1/3 < MEF VDAC2-. In the presense of redox-cycling compounds (menadione, lucigenin, nitrofurantoine), which are capable of receiving electrons from NAD(P)H dehydrogenases and transmit them to oxygen, the suppression of different VDAC isoforms also stimulated ROS production. This, at least in part, can be explained by the decrease of radical scavenging efficiency of cytochrome c/cytochrome c oxidase system. With use of original DBA-based fluorescent assay of NAD(P)H-oxidoreductase activity it was shown that VDAC1/3 and VDAC2 knockout lead to the decrease of activity of some non mitochondrial NADH-oxidoreductases, which, however, can be functionally associated with mitochondria.

Furthermore, increased expression of NADPH oxidases, including prosurvival NOX4 isoform D, was observed in MEF VDAC2- cells. Thus VDAC isoforms renders complex effect on the NAD(P)H oxidoreductase activity, ROS (and radical) production and utilization in cell. However, we were unable to reveal the own oxidoreductase activity of different VDAC isoforms.

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Voltage Dependent Anion Channels, ATP/ADP Exchange and Warburg Metabolism

ABSTRACT

Cancer cells express three VDAC isoforms. In tumor cells, high cytoplasmic free tubulin inhibits mitochondrial metabolism and membrane potential ($\Delta\Psi$) generation. When spindles form as proliferating cells enter metaphase, free tubulin decreases, and VDAC may open to better provide for the high ATP demands of cell division. We propose that relative closure of VDAC by tubulin together with non-electrogenic ATP/ADP exchange contributes to lower cytosolic ATP/ADP ratios, activation of aerobic glycolysis and a Warburg metabolic phenotype in proliferating cells.

KEYWORDS

Voltage Dependent Anion Channel, Warburg effect, anaerobic metabolism.

ACKNOWLEDGEMENTS

The work was supported by the grant of Government of the Russian Federation №14.Z50.31.0028.

SUMMARY

High rates of aerobic glycolysis and suppression of mitochondrial metabolism characterize the Warburg metabolic phenotype of cancer cells. During mitochondrial metabolism, hydrophilic metabolites like ATP, ADP, Pi and respiratory substrates enter and exit mitochondria through voltage-dependent anion channels (VDAC) in the mitochondrial outer membrane. Previously considered to be constitutively open, emerging data shows that VDAC is an adjustable limiter (governator) of mitochondrial metabolic flux. Rostovtseva and coworkers first showed that unpolymerized heterodimeric tubulin inhibits conductance of VDAC reconstituted into planar lipid bilayers. In tumor cells, high cytoplasmic free tubulin also inhibits mitochondrial metabolism and membrane potential ($\Delta\Psi$) generation. Cancer cells express three VDAC isoforms, and knockdown studies show that tubulin inhibits VDAC1 and VDAC2 but not the less abundant VDAC3. When spindles form as proliferating cells enter metaphase, free tubulin decreases, and VDAC may open to better provide for the high ATP demands of cell division. In aerobic post-mitotic cells like cardiac myocytes and hepatocytes, high cytosolic ATP/ADP ratios (up to 100 times greater than mitochondrial matrix ATP/ADP) is made possible by the electrogenic adenine nucleotide translocator (ANT) in the mitochondrial inner membrane, which exports $ATP4^-$ in exchange for cytosolic ADP^{3-} driven by $\Delta\Psi$. However in proliferating cancer cells, recent studies support the conclusion that non-electrogenic ATP/ADP exchange, possibly catalyzed by the ATP/Mg-Pi carrier, replaces electrogenic ANT exchange. We propose that relative closure of VDAC by tubulin together with non-electrogenic ATP/ADP exchange contributes to lower cytosolic ATP/ADP ratios, activation of aerobic glycolysis and a Warburg metabolic phenotype in proliferating cells.

ADDITIONAL INFORMATION

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Psychophysiological indices of reading skills in adults with a history of early psychosocial deprivation

SCIENTIFIC ORGANIZATION

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ABSTRACT

Our study investigated orthographic processing in adults who grew up in institutional care settings and individually-matched controls by analyzing a set of event-related potentials elicited during the lexical decision task that contained several experimental conditions, including legal orthographic strings (words), symbol strings (false font), legal pseudowords, and illegal non-words, aimed at eliciting specific neural responses (i.e., the N1 component).

KEYWORDS

ERP, language development, literacy, reading skills, institutionalization.

ACKNOWLEDGEMENTS

This research is supported by the grant from the Government of Russian Federation №14.Z50.31.0027.

SUMMARY

Most of children left without parental care in Russian Federation reside in institutional settings that are characterized by suboptimal levels of stimulation and early care. Existing body of research shows that early institutionalization is associated with a cascade of negative effects on children's development in a variety of developmental domains, including detectable alterations in brain structure and functioning (e.g. Nelson, Fox, & Zeanah, 2014). However, to the best of our knowledge, there are currently no published studies that examine the long-term effects of early institutionalization on the neural indices of literacy development and reading.

Our study tested the hypothesis that individuals who grew up in institutional care settings demonstrate altered trajectrories of spoken and written language development, in particular in the domain of literacy, which includes both writing and reading skills. This hypothesis is rooted in a) the observations of delayed language development and lower academic achievement of children raised in institutional settings, compared to their peers raised in biological families, and b) the complexity of reading as a multidimensional set of skills that relies on the complex interplay between linguistic, visual, phonological, motor, and cultural factors (e.g., Massaro et al., 1994, Dehaene, Cohen, Morais, & Kolinsky, 2015).

For example, recent evidence suggests that reading ability is correlated with efficiency of early visual processing, including repetition suppression and exemplar discrimination in the left occipital-temporal region known as the visual word form area — VWFA (Cohen et al., 2002; Ludersdorfer et al., 2013). This activity can be linked to letter-specific processing also revealed in the N1 (or N170) event-related potential (ERP; Pegado et al., 2014), and has been hypothesized to be sensitive to reading exposure and the development of fine print tuning.

Our study investigated orthographic processing in adults with a history of institutionalization and individually-matched controls (accounting for age, gender and SES) by analyzing a set of event-related potentials elicited during the lexical decision task that contained several experimental conditions, including legal orthographic strings (words), symbol strings (false font), legal pseudowords, and illegal non-words, aimed at eliciting specific neural responses (i.e., the N1 component).

The sublexical orthographic properties of words include general attributes of the writing system such as sequential dependencies and letter position frequencies. We focused on the ERPs that indexed sublexical orthographic effect through the difference in the amplitude of the N1 response to to pseudowords (orthographically legal) and non-words (containing illegal bigrams). In addition, we examined coding of orthographic information at the whole-word level that is based on the ability to represent the unique array of letters that defines a printed word (Araújo et al., 2015).

At the time of the writing of this abstract, our data collection was still in progress. We will present the preliminary findings regarding group differences in print tuning and orthographic processing between adults with and without history of early institutionalization.

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Increased hippocampal seizure susceptibility in FASD

SCIENTIFIC ORGANIZATION

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ABSTRACT

FASD - is common term used to describes the range of adverse developmental outcomes that may occur in a person whose mother drank alcohol during pregnancy and it's associated with several comorbidities including epilepsy. The mechanisms underlying epileptic phenomena associated with FASD are not fully understood. Here, we show increased excitability in hippocampal slices of the rats during the second postnatal week following single exposure to ethanol and identify the impairments in GABAergic inhibition that are likely involved in this increased excitability.

KEYWORDS

FASD, seizure, hippocampus.

SUMMARY

Fetal alcohol spectrum disorders (FASD) - is common term used to describes the range of adverse developmental outcomes that may occur in a person whose mother drank alcohol during pregnancy. FASD is associated with several comorbidities including epilepsy. Seizures are observed with a frequency of 3–21% in children with FASD. The mechanisms underlying epileptic phenomena associated with FASD are not fully understood. Here, we show increased excitability in hippocampal slices of the rats during the second postnatal week following single exposure to ethanol and identify the impairments in GABAergic inhibition that are likely involved in this increased excitability. Using extracellular recordings we observed that hippocampal slices prepared from the P7-9 rats 12 hours following alcohol exposure (6 g/kg, i.p.) display clonic-like and tonic-clonic seizure like activity during exposure to elevated extracellular potassium (6 mM) much more frequently than slices prepared from the control animals. Whole-cell recordings from CA3/CA4 pyramidal cells revealed strong reduction in the frequency of the GABAergic postsynaptic currents, without any change in their amplitude and kinetics, in slices from the ethanol-exposed animals. In parallel experiments in GAD-GFP P7-9 mice, we observed massive apoptosis, revealed with cleaved caspase-3 staining, in the hippocampal interneurons twelve hours following alcohol exposure. Thus, death of hippocampal interneurons following alcohol exposure may lead to impairments in GABAergic inhibition and increased seizure excitability in FASD.

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Advances and Challenges of Regenerative Medicine

SCIENTIFIC ORGANIZATION

Laboratory of Bioengineering and Regenerative Medicine (BioReM), Kazan Federal University

ABSTRACT

Regenerative medicine, including tissue engineering and cell therapy, is a promising field. Extensive research has been done on biological and synthetic scaffolds. Cell therapy has also been examined in experimental disease models and initial clinical transfer realized in patients with acute lung disease. There are a number of new possibilities at the early stages:regenerative potential of exosomes and proteosomes, 2D and 3D chip technology, organogenesis. However, further efforts are necessary to detect underlying mechanisms and the real impact for the treatment.

KEYWORDS

Regenerative medicine, tissue engineering, cell therapy, scaffold,organogenesis, exosomes.

SUMMARY

Regenerative medicine, including tissue engineering and cell therapy, is a promising and growing field. It has enormous potential to revolutionise medical treatment options for a very wide range of patients, such as those suffering from traumatic injuries, congenital defects, and simple aging and loss of function of organs and tissues.

Various tissue engineering approaches must be thoroughly tested and evaluated. Already extensive and successful research has been done on biological scaffolds, using donor organs that have been decellularized (using DNase, deoxycholate, SDS) and then reseeeded with the patient's own cells. Similarly research is ongoing into using synthetic scaffolds (fabricated using molding techniques, electrospinning, 3-D-printing) seeded with different cell types (MSCs, MNCs, epithelial cells, chondrocytes). Cell therapy has also been examined in experimental disease models and initial clinical transfer realized in patients suffering from acute lung disease. In addition to these approaches, there are a number of exciting new possibilities currently at the early stages of research, such as investigating the regenerative potential of exosomes and proteosomes, the uses for 2D and 3D chip technology, the formation of new organs through organogenesis and 3D bioprinting.

Small and large animals models have been used to generate both biological and synthetic tissue engineered grafts for the trachea, lungs, esophagus, heart, heat valves and the diaphragm. Initial clinical transfer of both has been performed for the trachea and oesophagus. Tissue engineered scaffolds for the trachea, the oesophagus and the diaphragm have been demonstrated their functionality in animal models. Early clinical data (5-year follow-up) provides initial evidence for successful tracheal and oesophageal replacement using biological scaffolds. Cell-based therapy has resulted in significant improvement in acute and chronic lung diseases both in experimental studies and clinical setting.

Regenerative medicine may represent a promising therapeutic alternative in the future. However, further efforts are necessary to detect underlying mechanisms and investigate the real impact of these new approaches for the treatment of thoracic diseases. These studies require careful consideration of the ethical issues to ensure that both in vivo and clinical research is carried out to give the maximum benefit to current and future patients with the minimum risk to human welfare and sacrifice of animal life.

Markova Svetlana

PhD

Senior Scientist

Copepod Luciferases: Properties and Application as Bioluminescent Reporters

SCIENTIFIC ORGANIZATION

Institute of Biophysics, Russian Academy of Sciences, Siberian Branch

ABSTRACT

Secreted luciferases of marine copepods are relatively small proteins ranging from 18.4 to 24.2 kDa that catalyze the oxidation of celenterazene to produce a bright blue bioluminescence. The first cloned copepod luciferases, GLuc from Gaussia princeps and MLuc from Metridia longa are successfully applied as extremely sensitive bioluminescent reporters for biological and medical research including in vivo imaging. But the search for bioluminescent reporters with more advanced properties is continued.

KEYWORDS

Bioluminescence, cloning, molecular evolition, protein structure, bioluminescent reporter, bioimaging, drug discovery.

ACKNOWLEDGEMENTS

This work was supported by by the Program of the Government of the Russian Federation "Measures to Attract Leading Scientists to Russian Educational Institutions" (grant 11.G34.31.0058).

SUMMARY

Secreted luciferases of marine copepods are relatively small proteins ranging from 18.4 to 24.2 kDa that catalyze the oxidation of their substrate, coelenterazine, to produce a bright blue bioluminescence.Highly homologous *Gaussia* and *Metridia* luciferases are the best known representatives of copepod luciferases. These luciferases share no sequence identity with other coelenterazine-dependent luciferases cloned to date, such as of *Renilla-, Oplophorus*-, and *Cypridina*-type. Today, the first cloned copepod luciferases, GLuc from *Gaussia princeps* and MLuc from *Metridia longa* are successfully applied as extremely sensitive bioluminescent reporters for biological and medical research including in vivo imaging. But the search for bioluminescent reporters with *more* advanced properties is continued.

With cDNA functional screening applied, we have shown that luciferase of *Metridia longa* is represented by multiple isoforms that were categorized into four types based on sequence features. Presumably, each type represents a separate non-allelic group of luciferase genes. These groups of MLuc isoforms differ in length (18.4 – 23.9 kDa) and share 53%, 68%, and 80% protein sequence identity with the group of luciferases having the longest sequences. The sequence alignment of the *M. longa* luciferase isoforms has shown a variable N-terminus of approximately 1/3 in length of the longest sequence followed by the conserved C-terminal region consisting of two non-identical repeats of ~70 amino acids. Each repeat contains highly conserved short motif of 32 amino acids with five highly conserved Cys residues suggesting the presence of up to 5 disulfide bonds per the protein molecule. These repeats of ~70 amino acids of *M. longa* luciferase expressed separately didn't reveal any bioluminescent activity. Only entire conserved C-terminal domain displays bioluminescence activity. The variable N-terminus is not important for bioluminescence because MLuc variant with truncation of this region retains the activity.

Some bioluminescent properties of different types of MLuc isoforms of different types and GLuc were investigated using recombinant proteins produced in baculovirus/insect cell expression system. All investigated luciferase isoforms display a very high bioluminescent activity and extreme thermostability retaining up to 70% activity after 30-min incubation at 100°C. The most significant differences were found in kinetics, salt concentration requirement, and specific bioluminescence activity. In addition, the temperature optimum of bioluminescent reaction ranged from extremely low 4°C to 20°C. It is highly probable that such different properties of the luciferase isoforms provide adaptability of copepod *M. longa* to rapid change of environmental conditions during diurnal vertical migrations. It also suggests that these isoforms of different luminescence properties may have different applications depending on experimental tasks.

Mikhailova Darya

Asessor Vineland adaptive behavior scale

Adaptive behavior of children in babyhomes with different social environment

SCIENTIFIC ORGANIZATION

Saint-Petersburg State University

ABSTRACT

We have conducted the investigation on how adaptive development of children in a family-liae environment is different from those characteristics of children in a typical socially-emotionally depriving babyhome. The study involved 52 infants (5-48 mounts, M = 23,06; σ = 9,93) and young children living in the two baby homes of St. Petersburg. To assess the health and functional abilities of children we used the expert evaluation method. To measure adaptive behavior a semi-structured interview «Vineland Adaptive Behavior Scale » (S. S. Sparrow, D. V. Cicchetti, 2005) was used.

KEYWORDS

Adaptive behavior, early age children, babyhomes, institutionalization, social environment, family environment.

SUMMARY

Early childhood period in life of every child is the basis for the development of personality and mental health. Difficulties in the child's early experiences such as deprivation, disregard, abusive treatment may be predictors of behavioral disorders and mental health problems. Understanding of the adaptive behavior of young children living in different conditions of social environment will allow us to understand which aspects of adaptive behavior unfold in a family environment. In its turn, that will improve intervention programs aimed at developing family environment in babyhomes. We have conducted the investigation on how adaptive development of children in a family-liae environment is different from those characteristics of children in a typical socially-emotionally depriving babyhome. The study involved 52 infants (5-48 mounts, M = 23,06; σ = 9,93) and young children living in the two baby homes of St. Petersburg. To assess the health and functional abilities of children we used the expert evaluation method. To measure adaptive behavior a semi-structured interview «Vineland Adaptive Behavior Scale » (S. S. Sparrow, D. V. Cicchetti, D.A. Balla, 2005) was used. Statistical methods: MANOVA, MANCOVA, correlational analysis, T-test. The results showed that children in the baby home with a family social environment have better developed personal and domestic daily living skills, social skills of interpersonal relations, play and coping skills, as well as expressive communication. Their development is better on three out of four domains, i.e. on Communication, Socialization and Daily Living Skill compared to children in a typical babyhome. Our data shows the importance of a family-like environment on the development of childrens social skills and proves the necessity to provide such environment for children in institutions.

Munzarova Alina
PhD student

A new method for accurate measurement of poleward microtubule flux in metaphase spindles of Drosophila S2 cells

SCIENTIFIC ORGANIZATION

Institute of Molecular and Cellular Biology SB RAS, Novosibirsk, Russia

ABSTRACT

The microtubule (MT) flux is the poleward movement of spindle MTs caused by their plus end polymerization coupled with minus end depolymerization. The flux regulates both spindle assembly and anaphase chromosome movement. We developed the "double spindle photobleaching (DSP)" method for measuring the flux in Drosophila S2 cell spindles containing Cherry-tagged MTs. This method allows a reliable measure of the flux rate over a 2-3-fold longer time than the standard photobleaching-based methods.

KEYWORDS

Mitotic spindle, microtubule flux, FRAP, Drosophila.

SUMMARY

The spindle is a highly dynamic microtubule (MT)-based machine that mediates chromosome segregation during mitotic and meiotic cell division. One of the dynamic parameters that characterize the spindle is the poleward MT flux, namely the continuous translocation of MTs toward the spindle poles caused by MT polymerization at plus ends coupled with depolymerization at minus ends. Poleward MT flux is observed in all higher eukaryotes and contributes to the regulation of spindle length and anaphase chromosome movement. One of the standard methods to assess the flux rate consists in generating a photobleached area across a spindle that contains fluorescently-tagged MTs, and then measuring the velocity of the poleward movement of the non-fluorescent stripe. However, this method only permits rapid measurements of the flux, because the fluorescence of the bleached stripe recovers rapidly due to the spindle MT turnover. Here we describe a modification of the current "single stripe photobleaching (SSP)" method for flux measurement. We photobleached two large areas at the opposite sides of the metaphase plate in *Drosophila* S2 cells expressing Cherry-tagged tubulin, leaving unbleached only the area near the chromosomes. We then measured the speed with which the fluorescent MTs move towards the poles. We found that this "double spindle pho-

tobleaching (DSP)" method allows a measure of the flux over a 2-3-fold longer time than the SSP method, providing a reliable evaluation of the flux rate.

ADDITIONAL INFORMATION

Co-autors: Alina Munzarova, Julia Popova, Alena Razuvaeva, Victor Shloma, Maurizio Gatti and Leonid Omelyanchuk

Murueva Anastasiya
PhD

Polymeric micro- and nano-scale systems as a platform for encapsulation and delivery of drugs based on resorbable polyhydroxyalkanoates

SCIENTIFIC ORGANIZATION

Institute of Biophysics SB RAS

ABSTRACT

During the implementation of mega-grant "Biotechnology of new biomaterials " the scientific basis for the development of drugs formulations with prolonged action based on PHAs was received. Micro- and nanoparticles were prepared from different types of PHAs. The experiments showed that by varying the technique of preparation and chemical composition of PHAs, one can prepare microparticles with different properties, which would be suitable for drug loading. The all PHAs used in this study are biocompatible and suitable for biomedical use.

KEYWORDS

Biomaterials, drug delivery system, polyhydroxyalkanoates.

SUMMARY

A drug delivery system (DDS) is defined as a formulation or a device that enables the introduction of a therapeutic substance in the body and improves its efficacy and safety by controlling the rate, time, and place of release of drugs in the body. Such systems are especially actual for treatment oncological and long current infectious diseases. Perspective material for creation such system are polyhydroxyalkanoates (PHAs). These polymers are biocompatible and inert towards animal tissues; in biological environments they are degraded to end products (CO_2 and H_2O). Investigations performed at the Institute of Biophysics, Siberian Branch, Russian Academy of Sciences and Siberian Federal University, revealed the high biocompatibility of high purity PHA samples at cellular and tissue levels, including contact with blood, as well as their applicability for the design of endoprostheses of various kinds, as matrices of functioning cells, and for deposition of drugs (Shishatskaya et al., 2008; 2011)

Work carried out in the framework of the mega-project, implemented under the supervision of leading scientists MIT professor "Biotechnology of new biomaterials" (USA) Anthony John Sinskey (RF Government Resolution № 220 of April 9, 2010), as a result of which it was possible to carry out comprehensive studies, including the development and optimization of methods for manufacturing micro- and nanoparticles from PHA by emulsion and spray-drying methods; research and identification of key factors influencing to the performance of engineered particles. Studying of the possibility of loading the wide range of drugs (cytotoxic, antibacterial and anti-inflammatory drugs) and the drug release in vitro. Research biocompatibility and adhesive properties of PHA microparticles with the assessment of the drug effectiveness of developed microcarriers.

Preparation and characterization of PHAs micro- and nanoparticles

The effect of the preparation technique (chemical composition of a polymer, type and method of emulsion mixing, and molecular mass of a drug) on the yield, structure, and size of microparticles obtained from resorbable polyesters of microbiological origin, polyhydroxyalkanoates, is studied. Microparticles made from degradable polyhydroxyalkanoates of different chemical compositions a homopolymer of 3-hydroxybutyric acid, copolymers of 3-hydroxybutyric and 4-hydroxybutyric acids (P3HB/4HB), 3-hydroxybutyric and 3-hydroxyvaleric acids (P3HB/3HV), 3-hydroxybutyric and 3-hydroxyhexanoic acids (P3HB/3HHx) were prepared using the solvent evaporation technique, from double emulsions. The present study re-

vealed a significant effect of the chemical composition of the polymer on the average diameter and ξ-potential of microparticles. It is found that the concentration of the polymer solution and the method of emulsion mixing are the most significant factors affecting the diameter of microparticles based on polyhydroxyalkanoates; the surface structure of particles depends to a higher extent on the chemical composition of the polymer. The family of microparticles from 100–200 nm to 50–70 μm in diameter is synthesized. This study showed that the values of ξ-potential of microparticles prepared from different types of PHAs varied significantly. The lowest values of ξ-potential were recorded for PHB3/HHx microparticles (-32.2 mV) and the ξ-potential of P3HB was no higher than -11 mV. Also, the possibility of using the spray drying method for the construction of PHA based microparticles was studied. The dependence of characteristics of microparticles (yield, average diameter, zeta-potential) from processing parameters (temperature at the inlet of the system, the feed rate of polymer solution and concentration of the polymer solution) was found. It is shown that zeta potential of microparticles was influenced by concentration of the polymer solution, and the average diameter was determined by temperature of the inlet. The zeta-potential of microparticles prepared by spray drying method was lower (from -66 to -115 mV) than that of P3HB particles. The conditions of obtaining P3HB microparticles were optimized to minimize polymer loss.

It were prepared microparticles loaded with different drugs. The study investigates properties of microparticles prepared from PHAs depending upon the method of preparation employed and taking into account the size of particles maintained in liquid media.

It is shown that the rate of drug release from microparticles in vitro into the medium is higher in the case of 3-hydroxybutyrate copolymers with 3-hydroxyvalerate than in the case of the homopolymer of 3-hydroxybutyrate. This parameter increases with the content of 3-hydroxyvalerate units in the copolymer and the porosity and mass fraction of the drug in particles with a decrease in their sizes. For in vitro systems containing a phosphate buffer, variation in the preparation parameters makes it possible to obtain microparticles with various characteristics suitable for deposition of drugs. For microparticles obtained from polyhydroxyalkanoates and having different diameters, the mathematical description of the kinetics of drug release from the polymer matrix is provided. The value of ζ-potential was influenced by drug loading into microparticles; the drug loaded microparticles maintained in balanced phosphate buffer for 30 days had higher physical stability than those without drug loading.

Biocompatibility and adhesive properties of PHA microparticles in vitro

In this study mouse fibroblast NIH 3T3 cells were cultivated on PHA microparticles, and results of using fluorescent DAPI DNA stain, and MTT assay showed that microparticles prepared from PHAs of different chemical compositions did not exhibit cytotoxicity to cells cultured on them and proved to be highly biocompatible. At 3 d after seeding, counts of attached cells showed that the number of cells on microparticles treated with H_2O_2 plasma was higher. The largest number of cells (up to 28-33 in the field of view) were attached to microparticles prepared from P3HB and P3HB/3HV with 20 mol% 3HV. That number was 1.4 – 1.8 times higher than the number of cells attached to the microparticles sterilized by autoclaving. The number of cells attached to autoclaved microparticles prepared from P3HB/3HV (6.5, 10 and 37 mol% 3HV), P3HB/3HHx, and P3HB/4HB (6.1 and 16 mol% 4HB) was half that recorded on the corresponding microparticles treated with H_2O_2 plasma. A possible explanation for this might be that treatment of polymer devices by physical methods (laser cutting or plasma) strengthens interphase adhesion joints, increasing surface hydrophilicity and, hence, improving its adhesion properties. MTT assay did not reveal any cytotoxic effect of autoclaved or plasma-treated PHA microparticles. The number of viable cells adhering to the surface of the matrices treated with H_2O_2 plasma was higher than on the surface of the autoclaved ones in all treatments. On plasma treated microparticles prepared from PHAs with different chemical composition, cells spread well and formed a monolayer. On the corresponding PHA microparticles sterilized by autoclaving, the number of cells was 1.5-2 times lower, and they showed an irregular shape. As differences in the number of cells proliferating on microparticles prepared from PHAs of different types are insignificant, all of the polymers investigated in this study are of good quality, showing high biocompatibility.

Different sized PHBV micro/nanospheres were tested for their effect on cell proliferation using L929 mouse fibroblasts and the MTT test. No significant effect of particle size on proliferation was observed. The effect of particles on cell proliferation was significant when the particle concentration was higher. These cells did not

show a change in their shape implying that the decrease is not due to a negative effect like toxicity which could have been observed by light microscopy.

Initial studies of particle penetration into the cells were carried out with the three batches of particles with different sizes. It was show that the cells take up the low and mid nano sized particles. An interesting finding was that the nanospheres were generally located in the cytoplasm near the nuclei. The larger (submicro) particles however, seemed to be unable to penetrate into the cells.

An in vitro study of the inhibiting effect of DOX-loaded microparticles

The cytostatic drug encapsulated in P3HB/3HV microparticles has been proven to be effective against HeLa tumor cells. At implementation of smaller particles (0.2 microns) with the highest load (0.6 μg /ml) the effect of the cytostatic drug depositing is comparable with free form as by the time of beginning of the action, so by the inhibiting effect on the cells. Particles loaded with the medium and lowest concentration (3.2 and 6.0 μg /ml) inhibited the growth of tumor cells only by the 3rd day of the experiment comparable with free DOX, but the beginning of the drug's action was late in time; the maximum inhibiting effect was observed on the 4^{th} day. This is connected with the kinetics of the drug outflow from the polymer matrix into the culture at which in the first two days the release of the drug in the culture was low (at the level 0,09 μg /ml and 0,07 μg /ml for the highest and the lowest concentration of DOX, correspondingly) and this concentration was insignificant for suppression of HeLa growth.

At implementation of larger polymer particles the effect of DOX depositing was more expressed. Delay in the inhibiting effect was registered only on the first day and only for the lowest and medium concentration of DOX (correspondingly, concentration of DOX in the culture made 0.08 μg /ml and 0.28 μg /ml). Nevertheless, already on the second day the cytostatic effect of the deposited DOX was comparable with the action of the free drug.

These findings demonstrated the efficiency of the cytostatic drug deposited in the microparticles conctrusted from resorbing polymers in relation to the culure of HeLa tumor cells.

Polymeric microcarriers loaded with anti-inflammatory substances in the therapy of experimental skin wounds

Development of effective preparation for the treatment of damaged skin serves as an actual problem of reparative medicine, which is related to a constant increase in the number of skin lesions due to burns, injuries, and surgical treatment.

Here we developed and tested a pharmaceutical form, degradable microparticles with anti-inflammatory substances, for the treatment of experimental skin lesions. We studied the effects of anti-inflammatory substances incorporated in polymeric microparticles made of degradable natural polyhydroxyalkanoate polyesters on experimental skin wounds caused by chemical burns in laboratory animals. Treatment with encapsulated forms of anti-inflammatory substances (applied in gel) accelerated wound healing in comparison with routine therapy (estimated by area of burn wound, wound healing activity, number of acanthotic cells, and number of hair and sebaceous follicles). The results showed the perspectives of usage of developed form of substances (degradable polymeric microparticles) for treatment of skin defects. Microscopy of the damaged skin showed that on days 2-4 of therapy, the histological pattern was similar in all groups. Edema of all dermal layers, inflammatory cell infiltration, disseminated focal necrosis in all dermal layers, and spasm of small vessels were found. Thus, the effects of free and encapsulated agents were similar. However, reparative processes in the skin (area of burn wound, intensity of wound healing, number of acanthosis cords, hair follicles, sebaceous glands, and horny cysts) in animals receiving microparticles were more pronounced. It should be noted that standard ointment compresses with the test agents were put daily for 11 days during the therapy, and applications of microparticles were made once at 3 days. Our results demonstrate positive effects of polymeric PHA-based microparticles with anti-inflammatory agents used as long-acting drugs for restorative treatment of skin lesions.

Study of the Efficiency of Doxorubicin Deposited in PHAs Microparticles on Laboratory Animals with Ehrlich's Solid Carcinoma

We also have studied the antitumor effects of doxorubicin, encapsulated in PHA matrix, towards Ehrlich's solid carcinoma (EC). Use of the experimental form of the cytostatic in polymeric microparticles from resorbable PHAs in animals with solid

tumor led to inhibition of the cancerous process, comparable to that in response to intravenous free doxorubicin, but without negative effects on the blood system. No negative effect of injection of microparticles charged with doxorubicin was recorded. Blood analysis showed no changes beyond the normal range of values or appreciable differences in comparison with intact animals. Group animals (free doxorubicin) developed a 2-fold reduction of the leukocyte count by the end of experiment. This was presumably caused by the antibiotic toxicity for hemopoietic organs.

Formation of slit-like necroses in tumor tissue was found in all groups after 1 week. In the positive control group, the necroses occupied large fields close to the central part of the tumor, the tumor tissue was retained at the periphery, in zones of infiltrative growth. In experimental groups, the necroses were grouped in large fields in the central compartments, while smaller ones were chaotically scattered at the periphery. The area of necrotic zones in experimental and positive control groups was about 30% of tumor tissue area. Two weeks after the beginning of therapy the antitumor effect was significantly higher in the positive control group than in experimental groups. However, after 3 weeks the maximum tumor growth inhibition (area of necrotic zones reaching 78% of tumor tissue area) was recorded in experimental group 5 (in response to double cycle dose of the drug). In group 3 animals (intravenous drug weekly) and in group 4 (a single cycle dose of the drug encapsulated in microparticles) the necrotic zones occupied 63-64% of tumor tissue area during this period; the values in these groups virtually did not differ. It is noteworthy that the necrotic zone area in the negative control group varied from 18 to 30% throughout the entire experiment.

Our experiments on the solid EC model demonstrated that PHAs was fit to serve as a doxorubicin carrier for local treatment and showed the antitumor efficiency of the drug encapsulated PHAs microparticles.

ADDITIONAL INFORMATION

Work was carried out with the participation of Doctor of Science E.I. Shishatskaya and PhD A.M. Shershneva.

Nasretdinov Azat
Researcher

Developmental EEG correlates of sleep and wakefulness in rats

SCIENTIFIC ORGANIZATION

Kazan (Volga region) Federal University

ABSTRACT

In the early postnatal period in rats, cortical activity is organized as alterations of network silence and activity bursts. Using simultaneous multichannel recording of cortical activity, EMG recording of nuchal muscle activity and video recording of animal's behavior we explore how the early cortical activity is modulated by distinct behavioral substates of sleep and wakefulness during development.

KEYWORDS

Electroencephalography, Barrel Cortex, Rat, Wakefulness.

SUMMARY

Short myoclonic twitches of limbs or entire body generate primary sensory cortex activation in neonatal rats contributing development of somatosensory system. Similar spontaneous muscle twitches observed also in whiskers system. Spontaneous whisker movements and patterns of cortical activity occuring during sleep well studied. However, it remains unknown how whisker movement activity organized in wake state and how it correlates with neuronal activity in primary somatosensory cortex during first postnatal week, when basic movement pattern of whiskers (whisking) has not been formed. During wake periods we observed slow oscillatory whisker movements in 2-5 Hz frequency called protowhisking. During each episode of wake movements we observed raising activity in somatosensory cortex in form of increased action potential frequency and spectral characteristics of local field potential.

Nedospasov Sergei

Doctor of Sciences, RAS Associate Member

Head of research laboratory

Cell type-restricted cytokine targeting in disease

SCIENTIFIC ORGANIZATION

Engelhardt Institute of Molecular Biology and Lomonosov Moscow State University, Moscow; Lobachevsky State University of Nizhny Novgorod

ABSTRACT

Using mouse models we are pursuing the idea of more selective neutralization of proinflammatory cytokines in disease that may have advantage over systemic blockade. This concept is supported by both genetic and pharmacological data.

KEYWORDS

Cytokine, autoimmunity, antibody, bioengineering.

ACKNOWLEDGEMENTS

Supported by grant 14.Z50.31.0008 from the Ministry of Education and Science of the Russian Federation and by grant 14-25-00160 from Russian Science Foundation.

SUMMARY

Proinflammatory cytokines, such as TNF and IL-6, contribute to pathogenesis of several autoimmune diseases with an inflammatory component. Systemic neutralization of these molecules is the basis for therapeutic intervention and has already made a revolution in medicine. Howeverm studies in experimental arthritis suggested that TNF from one particular cellular source may play a protective role. If so, systemic cytokine inhibition is a double-edged sword disrupting both pathogenic and protective signaling. On the other hand, in several disease models in mice TNF produced by myeloid cells is pathogenic. Based on these findings we have developed an approach to cell type-restricted cytokine neutralization. We are utilizing bispecific antibodies that would attach to the cell surface of a particular type of immune cells, and capture the cytokine released by these cells, preventing its systemic dissemination. Our inhibitors are based on single domain antibodies (VHH) specific for human or mouse TNF, human IL6 and for cell type-specific markers, in particular, for F4/80 surface molecule expressed on the surface of macrophages. We demonstrate that such antibodies can effectively attach to the cell surface, capture and retain the released cytokine. Using mice humanized for the TNF system and macrophages isolated from such mice we assessed activity of such bi-specific constructs in vitro and in vivo. Our findings indicate that macrophage-restricted TNF neutralization has advantages over systemic TNF inhibition, paving the way to bioengineering of a new type of cytokine inhibitors.

Nizamieva Aygul

Student

The influence of anisotropy on excitation wave propagation in neonatal rat cardiomyocytes monolayer

SCIENTIFIC ORGANIZATION

Moscow Institute of Physics and Technology

ABSTRACT

This work is devoted to various models of the cardiac arrhythmias and the modeling of the spiral wave formation, in particular. To create controlled anisotropy in a cultured cell layer for cardiac arrhythmias models we used a photosensitive agent AzoTAB. In this paper, two main models have been created: the model of unidirectional block and the model with a gradient of excitability. Also simulations were calculated theoretically on the Aliev-Panfilov model.

KEYWORDS

Azotab, photocontrol, arrythmia, optical mapping, heart disease, ablation.

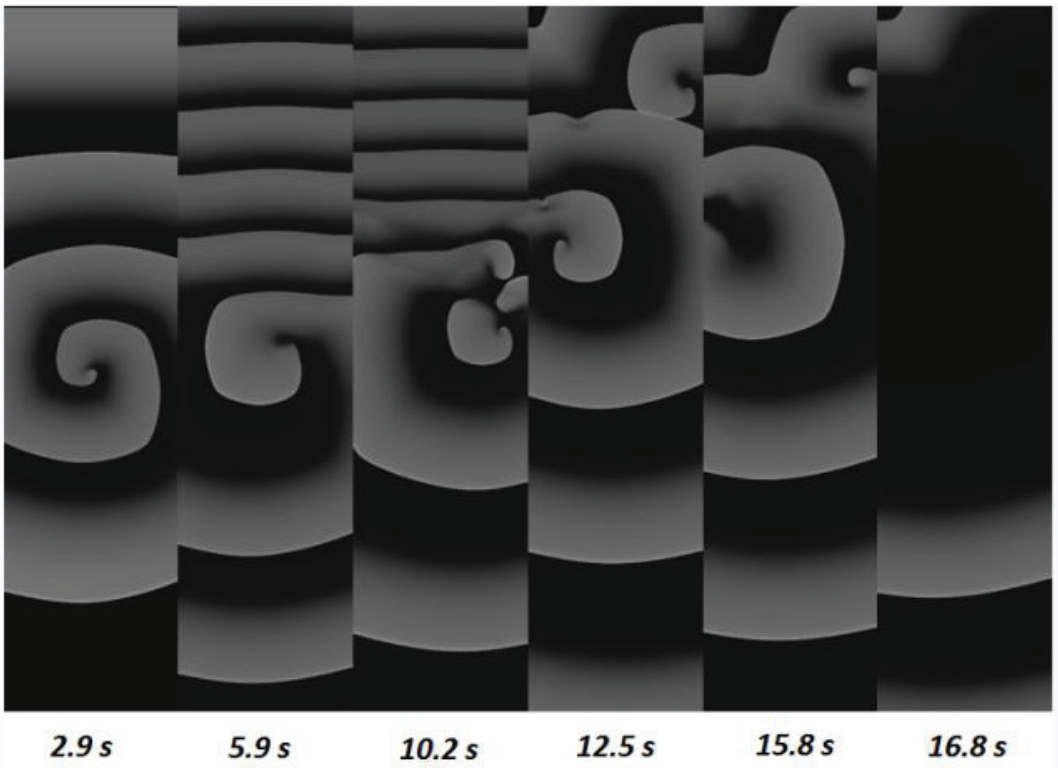
ACKNOWLEDGEMENTS

We thank our colleagues — Tsvelaya V., Kalita I., Kudryashova N.,— who contributed immeasurably to the work. We especially want to thank Agladze K.I.

SUMMARY

Cardiac arrhythmias are among the most common causes of death in the world, therefore studying mechanisms of their initiation is one of the priorities of modern science. This work is devoted to various models of the cardiac arrhythmias and the modeling of the spiral wave formation, in particular. To create controlled anisotropy in the cultured cell layer for cardiac arrhythmias models we used a photosensitive agent of azobenzene-based compounds called AzoTAB ((2- {4- [(E) -2- (4-ethoxyphenyl) diazo-1-yl] phenoxy} ethyl) trimethylammonium bromide). In the dark, thermally relaxed state or in a state under blue light (λ> 440 nm) trans-AzoTAB reversibly reduces spontaneous activity and the rate of propagation of excitation waves until absolute blockade. Excitation waves may be renewed by near-UV irradiation (λ ≈ 365 nm), which converts AzoTAB to the cis-form. In this paper, two main models have been created: the model of unidirectional block and the model with a gradient of excitability.

The model of a unidirectional block relies on a creation of inhomogeneous excitability in the tissue. In areas irradiated by UV-light the activation threshold of excitation is lower compared to the non-irradiated or weaker irradiated areas, so in a presence of abrupt UV gradient (at certain concentrations of AzoTab) excitation wave passes from the non-irradiated area to the irradiated one and can't propagate in the opposite direction . This model is similar to the behavior of a semiconductor diode and describes the main mechanism for the formation of a circulating (spiral) wave. A modeling of of spiral waves drift in a gradient of excitability in the monolayer of cardiomyocytes is based on the critical degrees of excitation determined in the first model. For example, with 20%-intensive UV exposure the conduction velocity drops by 1.7 times compared to 100% exposure. Spiral wave, formed in such gradient of excitability, drifts more frequently towards lower excitability. Computer simulations employed Aliev-Panfilov model with the two-fold difference in speed have shown similar behavior of the rotating wave (figure 1).



Odinokova Irina
PhD
Staff scientist

Chronic ethanol feeding causes controversial changes of functional parameters of rat liver mitochondria

SCIENTIFIC ORGANIZATION

Institute of Theoretical and Experimental Biophysics of RAS

ABSTRACT

Chronic ethanol consumption causes liver disease and the earliest pathophysiological changes take place at the level of mitochondria. We studied the effect of chronic ethanol feeding on the parameters of rat liver mitochondria. We showed that chronic ethanol consumption decreased mitochondrial respiratory control ratio, but improved their ability to retain calcium and delayed mPTP opening. We suppose that changes in structural and/or regulatory components of mPTP could be an adaptive mechanism protected mitochondria from oxidative stress during chronic ethanol treatment.

KEYWORDS

Chronic ethanol consumption, liver mitochondria, mPTP.

ACKNOWLEDGEMENTS

This work was supported by grant of the Government of the Russian Federation № 14.Z50.31.0028 and grant of the Russian Foundation of Basic Research № 16-04-00927.

SUMMARY

Chronic ethanol expose is known to be associated with a range of liver disorders – hepatic steatosis, alcoholic hepatitis, hepatic fibrosis and cirrhosis. Some of the earliest pathophysiological changes take place at the mitochondrial level. We studied the effect of prolonged ethanol feeding on the parameters of rat liver mitochondria. Two groups of Wistar rats received Lieber-DeCarli liquid diet, where ethanol was added to yield a 5% (w/v) dose, and ethanol was isocalorically replaced with maltose/dextrin in control diet. Control rats were pair fed to their ethanol counterparts for 10 weeks. Experimental and control animals consumed 85-100 kkal per day and alcoholic rats received about 17 grams of ethanol per kg of body weight. The following mitochondrial parameters were measured: mitochondrial respiration, membrane potential, Ca^{2+} transport and mitochondrial swelling. We showed that rate of mitochondrial respiration of ethanol-fed rats increased at state 2 and decreased at state 3 leading to reduction in respiratory control ratio by 35%. Interestingly, Ca^{2+}-capacity of mitochondria isolated from ethanol rats increased, their membrane potential was more stable, and rate of mitochondrial swelling was decelerated. Thus, in our experiments we observed that mitochondria from ethanol-treated rats improved their ability to retain Ca^{2+} and mPTP opening was delayed, which is opposite to the literature data. We supposed that changes in structural and/or regulatory components of mPTP during chronic ethanol consumption could be the reason for the resistance of mitochondria to damaging conditions. Several mitochondrial proteins related to mPTP were tested using Western blot assay (subunit c of FoF1-ATPase, VDAC1, VDAC3, CNP, TSPO, Bcl-xL). It was found that level of subunit c of FoF1-ATPase was significantly increased in mitochondria from ethanol-fed rats, furthermore the level of phosphorylated form of subunit c was also higher in ethanol mitochondria compare to control ones. Earlier we showed that induction of mPTP opening in rat liver and brain mitochondria correlated with Ca^{2+} and CsA-sensitive dephosphorylation of subunit c of FoF1-ATPase and subunit c might be a structural or regulatory component of mPTP. Thus increase of phosphorylated subunit c level could be an adaptive mechanism protected rat liver mitochondria from oxidative stress during chronic ethanol treatment.

ADDITIONAL INFORMATION

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Photosensitizer loaded calcium carbonate particles for theranostics.

SCIENTIFIC ORGANIZATION

Saratov State University

ABSTRACT

Calcium carbonate is an important inorganic biomaterial thanks to its chemical stability, bioactivity, and biocompatibility, which made it an interesting candidate for drug delivery systems. We report on studies of photosensitizer loaded vaterite containers in cell culture assays, and in vivo biodistribution. The resultant uptake of particles demonstrated particles accumulation in the tumour was benchmarked as 0.43 of that in the liver. Such pharmacokinetics of vaterite particles holds promise for its deployment in drug delivery applications

KEYWORDS

Vaterite, particles, drug delivery, photosensitizer, photodynamic therapy, porphyrazine, molecular rotors.

ACKNOWLEDGEMENTS

This work was supported by grant 14.Z50.31.0022 for the porphyrazine synthesis, cell and animal studies. Grant 14.Z50.31.0004 supported the vaterite particle synthesis and microscopy.

SUMMARY

Calcium carbonate is an important inorganic biomaterial thanks to its chemical stability, bioactivity, and biocompatibility. These properties have recently made it an interesting candidate for drug delivery systems. Calcium carbonate exists in three anhydrous polymorphic modifications: vaterite, aragonite, and calcite. Under normal conditions, vaterite is an unstable phase, while calcite and aragonite are stable. Vaterite polycrystalline particles have further favorable properties like high porosity, large surface area, and negative zeta potential. We present a novel technique for the synthesis of CaCO3 containers. Porous polycrystalline particles were fabricated with controllable average sizes from 400 nm up to 10 microns. Several levels of control on these release dynamics could be identified: 1) The immersion medium: capsules immersed in water, showed a delayed burst release of the dye, coinciding with the crystal phase transition from vaterite to calcite. In ethanol this phase transition was inhibited, consequently only a slow desorption of the encapsulated dye was found. 2) Surface modification: Covering microcontainers with additional layers of biocompatible polyelectrolyte increases the payload release time. 3) pH value: A change of the pH from neutral to acid conditions will instead lead to a destruction of the vaterite matrix leading to an immediate release.

In current work we have demonstrated that vaterite particles were capable to load a substantial amount of anticancer photosensitizer drug porphyrazine. Porphyrazine is a molecular rotor whose fluorescence intensity and lifetime enabled fluorescence imaging and assessment of its rotation mobility in particles, cells and biological tissues.

In vitro and in vivo studies of the particles loading, cell uptake and particles bio distribution in organs were performed. After the one hour of incubation with the human breast adenocarcinoma cells the particles successfully penetrate through the cell membrane and predominantly localized in the cytoplasm.

For in vivo studies the loaded vaterite particles dispersed in buffer solution was injected intravenously in a wild-type mouse (Balb/c) bearing a grafted colorectal adenocarcinoma. The resulted accumulation of vaterite particles in the tumor was 0.4 respect to the in the liver. That have been confirmed via two methods: fluorescence whole-animal imaging and histology analysis. Such high tumor uptake efficiency possible explain via the enhanced permeability and retention. Flexible loading and release control mechanisms, the perfect biocompatibility and revealed pharmacokinetic have proven the system’s potential for future pharmaceutical applications.

ADDITIONAL INFORMATION

This work is result of collaborative research between two megagrant laboratories: Laboratory of optical theranostics (Lobachevsky Nizhny Novgorod State University, 603950 Nizhny Novgorod, Russia) and Remote controlled theranostic system lab (Institute of Nanostructures and Biosystems, Saratov State University, 410012 Saratov, Russia).

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SCIENTIFIC ORGANIZATION

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Genetic control of kinetochore-driven microtubule growth: An RNAi-based analysis in Drosophila S2 cells

ABSTRACT

To understand the mechanisms of chromosome/kinetochore-driven microtubule (MT) formation we analyzed MT regrowth after MT depolymerization in Drosophila S2 cells. MT regrowth assays were performed in cells subjected to RNAi against 10 individual spindle components. We identified factors that promote MT regrowth and factors that inhibit this process. Our results provide a sound starting point to develop a molecular model for the regulation of kinetochore-driven MT growth.

KEYWORDS

Drosophila S2 cells, mitosis, spindle, kinetochores, microtubule regrowth assay.

SUMMARY

Chromosome/kinetochore-driven microtubule formation is essential for proper spindle assembly. To dissect the mechanisms underlying this process we analyzed spindle microtubule (MT) regrowth after cold- or colcemid-induced MT depolymerization in *Drosophila* S2 cells depleted of individual spindle components. Specifically, we used RNAi to deplete 3 MT-destabilizing kinesins (Klp10A, Klp59C and Klp67A), 2 proteins that favor MT plus end growth (Eb1, Mast/Orbit/Clasp), 2 proteins that bind and stabilize the kinetochore fibers (Mars/HURP and Mei-38/TPX2), 2 proteins that specifically associate with the MT minus ends (Asp and Patronin), and Dgt6, a component of the augmin complex that mediates lateral MT growth from preexisting MTs. MT regrowth assays performed in prometaphase/metaphase cells showed that depletion of the MT-destabilizing kinesins does not affect kinetochore-driven MT growth, which is instead reduced by the loss of Eb1, Mast/Orbit, Mars, Mei-38 or Dgt6. Surprisingly, we found that depletion of either Asp or Patronin increases the rate of MT regrowth from the kinetochores. The current model on kinetochore-driven MT growth in cells not exposed to MT depolymerization suggests that kinetochores capture the plus ends of the MTs that form in their vicinity, and that polymerization of these plus ends leads to formation of kinetochore fibers with the minus ends pointing away from the chromosomes. Our results are consistent with this model and identify several factors that are necessary for growth and stabilization of the MT bundles emanating from the kinetochores. However, the precise roles of Asp and Patronin in the regulation of kinetochore-driven MT regrowth remain to be defined.

ADDITIONAL INFORMATION

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Optimization of detection method of monocyte-platelet complexes in whole blood

SCIENTIFIC ORGANIZATION

Moscow State University of Medicine and Dentistry named after A.I. Evdokimov

ABSTRACT

Despite the great clinical importance of intercellular complex formation in platelet activation, flow cytometric methods of their detection are poorly standardized. Many methods that reduce the contribution of in vitro platelet activation have been developed for enumeration of monocyte-platelet complexes (MPC). Technique of blood sampling, the choice of anticoagulant, methods of sample fixation, erythrocyte lysis have a significant effect on the percentage of the MPC, which differs according to different authors, from 3,72±1,39 up to 12,3±3,3% in the blood of healthy donors.

KEYWORDS

Monocyte-platelet complexes, flow cytometry.

ACKNOWLEDGEMENTS

This study was supported by the Grant of the of the Government of the Russian Federation, contract #14.B25.31.0016.

SUMMARY

Methods: The study included ten healthy volunteers. Peripheral venous blood was sampled by direct venipuncture to a 3.8% sodium citrate containing tube. Tubes were gently inverted to ensure mixing of whole blood with anticoagulant. Thirty microliters of whole blood (either fixed or unfixed) were immediately immunolabeled with 20 microliters of fluorescent monoclonal antibody mix (CD45-eFluor450, CD14-PerCP Cy5.5 and CD41a-APC, containing 2% of mouse IgG to prevent non-specific binding) for 20 minutes in order to identify monocyte-platelet complexes. Sample was diluted with 2 ml of phosphate buffer saline (PBS) or 2 ml of 0.5% formaldehyde and subjected to flow cytometry. Monocyte-platelet complexes were detected by simultaneous expression of all three markers. The MPC positive gate was defined based on fluorescence minus one control (FMO-IgG), including IgG1-APC (Figure 1).

Monocytes were labeled with CD45-eFluor450, CD14-PerCP Cy5.5 and platelets with CD41a-APC. Monocytes were gated based on their high expression of CD14 and presence of CD45 antigen. Minimum of 2 500 events was collected in the monocyte gate (A). Fluorescence minus one control, containing IgG1-APC isotype antibody was used to define double positive monocyte-

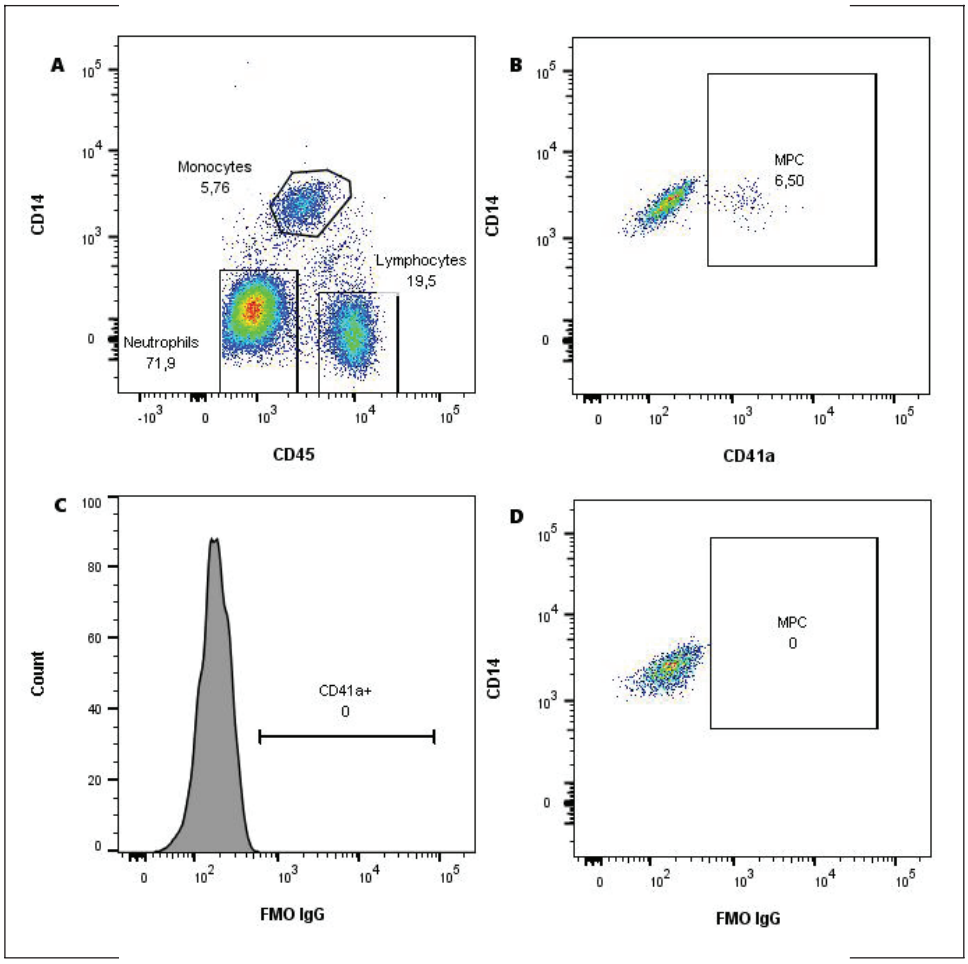

Figure 1. Flow cytometric analysis of monocyte-platelet complexes in mildly fixated whole blood

platelet complexes based on APC histogram(C) and dot plot (D) to set a marker excluding for non-specific binding and autofluorescence. Dot plot containing the pre-defined gate of double-positive CD14+CD41a+ then used to determine the percentage of monocytes positive fir CD41a (B).

The flow cytometric data was acquired at medium to high flow rate using CD45 threshold set on 200 to avoid collection of unwanted erythrocyte events.

Different sample processing protocols were utilized to identify the method that minimizes the in vitro cell activation and preserves most of the complexes, formed in vivo:

1. Whole blood samples were stained immediately (within 2 minutes) after collection for 20 minutes at room temperature and then fixed.

2. One hundred microliters of whole blood was immediately fixed with equal volume of cold formaldehyde solution resulting in different final concentrations (0.25-4%) before immunolabeling for 20 minutes .

2. Erythrocyte lysis was performed either after (using eBioscience RBC lysis solution) or simultaneously with cell fixation (using BD lyse reagent).

3. Whole blood sample pre-fixed with 0.25% formaldehyde was then stained and finally fixed with 2 ml of 0.5% formaldehyde.

4. The stability of MPC was assessed for the timeline of 24 hours at 4°C.

Results and discussion: The time from blood collection to the fixation of the sample is a critical factor which increases the number of MPC by in vitro cell activation. Staining of the samples for 20 minutes immediately after blood collection results in 35.4±3.5% MPC, and each 30 minute delay prior blood processing adds 20-25% of MPC. On the other hand, when samples are fixed immediately after blood collection, MPA content remains stable for a longer time. The concentration of the fixative also affects the MPA concentration. Higher formaldehyde concentrations (1-4%) change neutrophil and monocyte scatter properties and result in clumping of dead cells at 4%. Immunolabeling in high concentrations of formaldehyde (1-2%), although permanently stabilizes the cell membrane, reduces the fluorescence of the most fluorochromes.

Lower concentrations of methanol-free formaldehyde (0.5-0.25%) do not interfere with immunostaining and are able to temporarily stabilize the amount of MPC without reducing the level of fluorescence. The percentage of monocytes, complexed with platelets in mildly fixated whole blood of healthy donors is 6,5±2,2%.

Lysis of red blood cells leads to further activation of platelets and monocytes and increases complex formation, and therefore it is preferable to avoid it. The RBC lysis without fixation requires washing steps, which markedly affects the amount of MPC. Simultaneous lyse-no-wash protocol using commercially available reagents, containing 1% of formaldehyde bears the drawbacks of the high concentration fixation discussed above.

The samples fixed in 0.5% formaldehyde remain stable MPC content for 24 hours at 4°C.

Conclusions: The amount of monocyte-platelet complexes is an early marker of immunoactivation and atherothrombosis (Furman et al. 2001, Harding et al., 2007). However, the high sensitivity of the method, requires thorough optimization of the parameters of sample preparation and analysis, to obtain stable and accurate results in order to exclude in vitro platelet activation.

In this study we have developed a method of processing and analysis of monocyte-platelet complexes in whole blood, which minimizes the effects of in vitro activation of platelets and monocytes, allowing to quickly and effectively enumerate the percentage of MPC.

Additional information

This study was supported by the Grant of the of the Government of the Russian Federation, contract #14.B25.31.0016.

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Study of the alcohols influence on excitation wave propagation in neonatal rat ventricular myocyte monolayer

SCIENTIFIC ORGANIZATION

Moscow Institute of Physics and Technology (State University)

ABSTRACT

Cardiac arrhythmias are often associated with alcohol consumption. However, the underlying mechanism of alcohol induced arrhythmias still poorly known. In this study we show the effect of ethanol and heptanol on excitation wave propagation on the experimental heart model - neonatal rat ventricular myocyte (NRVM) monolayer by optical mapping method.

KEYWORDS

Optical Mapping, Arrhythmias, Reentry, Gap-junction, Ethanol.

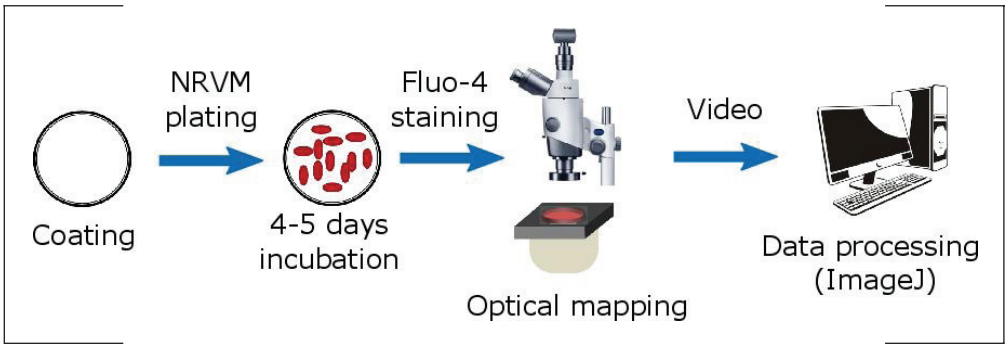
ACKNOWLEDGEMENTS

We thank all the colleagues from the Laboratory of the Biophysics of Excitable Systems of MIPT who provided insight and expertise that greatly assisted this research.

Summary

A wide range of chemical compounds and drugs has potential cardiotoxic effect which can result in cardiac arrhythmias. A special role in this case play alcohols. In medical research it is a known fact that the use of ethanol in large quantities causes cardiomyopathy and prolongs QT-interval [1]. In the experiments on isolated cells it was shown that the ethanol inhibits voltage-gated ion channels (fast sodium, L-type calcium channels and the transient outward potassium current) [2]. But a full picture of fundamental role of this substance in the cardiac functioning still does not exist. Heptanol is used in the electrophysiology as a gap junctions blocker [3,4]. In our study we put in a goal to evaluate effects of ethanol and heptanol on a cultured monolayer of cells - neonatal rat ventricular myocytes (NRVM).

Figure 1. The experimental scheme.



While increasing concentration of the alcohol, velocity of the excitation wave propagation and maximum capture rates were measured by optical mapping method. The experimental scheme is shown on Fig. 1.

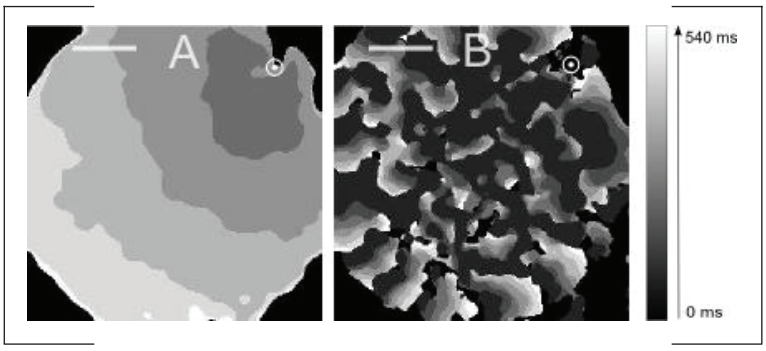


Figure 2. Activation maps of NVRM monolayer. A-control, B-0.9 mM heptanol. White point in the corner corresponds to the place of stimulating electrode. Scale 38 μm.

For both alcohols excitation wave propagation velocity decreases exponentially at concentrations from 0.05 to 1.8 mM. In experiments with heptanol conduction block was observed at 1.8 mM, which confirms its role in cells uncoupling. Notably, that in the interval between 0.4 and 0.6 mM of heptanol velocity locally rose by 20% comparing to the current values. It may indicate the activation of specific ion channels at these concentrations. On 0.1 mM the effect of heptanol accumulation with time was observed. The activation maps of NVRM monolayer with treatment of 0.9 mM heptanol/without treatment are given on Fig.2.

Unlike the ethanol, at high (0.8-1.4 mM) concentrations of which, excitation wave propagation velocity dropped 5-fold times comparing to normal conditions. Therefore, the length of propagating impulse decreased considerably. Consequently,

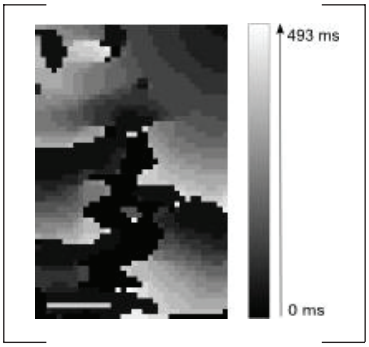


Figure 3. Activation map of NVRM monolayer with 1.4 mM ethanol treatment. Scale 12 μm.

the size required for the existence of reentry become significantly smaller (Fig. 3) [5]. This fact may represent pro-arrhythmogenic action of the ethanol.

Values of maximum capture rates also reduced with the increase of ethanol concentration: at 0.8-1.4 mM more than 60%. Maximum capture rate characterizes total duration of the action potential and refractory period, so its reduction with the increase of ethanol concentration is consistent with QT-prolongation data.

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SPAdes genome assembler

SCIENTIFIC ORGANIZATION

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ABSTRACT

Originally, we have developed a genome assembler tool (SPAdes) for the purpose of overcoming the complications associated with single-cell microbial data. Later, SPAdes was recognized by the scientific community as one of the best assemblers for bacterial data sets. This fact inspired us to extend the capabilities of SPAdes to include additional sequencing platforms (e.g. PacBio and Oxford Nanopore) and to develop a set of novel software tools for various purposes: assembly of highly polymorphic genomes, metagenome assembly, plasmid assembly, transcriptome assembly etc.

KEYWORDS

Sequencing, genomics, genome assembly, single-cell sequencing, metagenomics, transcriptomics.

ACKNOWLEDGEMENTS

The project was supported by the Government of the Russian Federation [grant numbers 11.G34.31.0018, 11.G34.31.0068], St. Petersburg State University [grant number 15.61.951.2015] and the Russian Science Foundation [14-50-00069].

SUMMARY

Despite all the efforts, *de novo* genome assembly is a complex task that so far remains unsolved. The assembler tool SPAdes [1, 2] was originally developed by the researchers from Center of Algorithmic Biotechnology (St. Petersburg State University) for the purpose of overcoming the complications associated with single-cell microbial data obtained via Multiple Displacement Amplification [3]. In contrast to conventional genome sequencing, this type of data is characterized by the uneven read coverage, increased level of errors and chimerical reads. SPAdes was able to successfully resolve these issues for Illumina reads and was recognized by the scientific community as one of the best assemblers working with both isolates and single-cell data [4]. Even though the assembler was specifically

designed to work solely with microbial genomes, scientists have tested the tool on a large number of different types of other data (e.g. metagenomic data, larger genomes etc). Their efforts and feedback have inspired us to extend the capabilities of SPAdes to include additional platforms (Ion Torrent, Pacific Biosciences, Oxford Nanopore, Illumina TruSeq), combinations of platforms, and to develop a set of novel software tools for various purposes: assembly of highly polymorphic genomes [5], metagenome assembly [6], plasmid assembly [7] and *de novo* transcriptome assembly from RNA-Seq data.

In this work we discuss the origin of single-cell bacterial sequencing and the main challenges in assembling such kind of data. We briefly describe the developed SPAdes pipeline and core algorithmic ideas that allowed us to successfully address the problem of *de novo* assembly using single-cell sequencing [2] and later to develop a set novel SPAdes-based tool for assembling various types of sequencing data [5, 6, 7, 8, 9, 10, 11]. In conclusion we discuss the current progress and future plans for assembly-related projects in our lab.

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ADDITIONAL INFORMATION

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Identification of the genetic cause for quadrupedal locomotion in human subjects by high- throughput sequencing

SCIENTIFIC ORGANIZATION

Center of Brain Neurobiology and Neurogenetics, The Federal Research Center Institute of Cytology and Genetics of Siberian Branch of the Russian Academy of Sciences

ACKNOWLEDGEMENTS

We thank Dr. Garcias and Dr. Roth who previously made clinical description of this case (Garcias and Roth, 2007) for help in collection of the specimens. The work was supported by the Government of the Russian Federation (Project №14. B25.31.0033, Resolution No.220 Federation of April 9, 2010).

SUMMARY

Rare form of autosomal recessive congenital ataxia with severe mental retardation, quadrupedal locomotion, absence of speech and signs of hirsutism was identified in Brazilian family with a consanguineous marriage. We performed convergent genetic analysis of affected descendants and their healthy relatives using Affymetrix Genome-Wide Human SNP Array 6.0 and a whole genome sequencing using Illumina platform. Microarray data analysis identified the set of homozygous genomic loci linked to the disease. In follow up whole genome sequencing we analyzed the homozygous regions and identified the large homozygous deletion disrupting one of the gene for putative neurotransmitter receptor.

To study evolution of the gene the protein–coding sequence of the gene across 43 species was examined by branch and branch-site specific models of Likelihood Ratio Test by PAML software. Next, non-coding elements conserved between the primates (phastConsElements46wayPrimates, UCSC tables) in 1 Mb region harboring the gene were examined by pairwise comparison using Tajima's Relative Rate Test included in MEGA software package. Our study revealed the genetic defect eliminating evolutionary conserved part of the gene leading to impairment of human-specific trait for locomotion and intellect and identified the trajectory of evolutionary changes of this gene in human lineage.

ADDITIONAL INFORMATION

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Development of blocking streptabody specific to CD47 receptor on cancer cells

SCIENTIFIC ORGANIZATION

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ABSTRACT

Development of high affinity molecules possessing the ability to block or modify the functional activity of receptors on the surface of cancer cells might have great application in perspective personalized therapy of tumor diseases. VHH antibodies and their various multivalent forms might be promising therapeutic agents. The aCD47cl19VHH-BAD antibody was obtained to create streptabody which might have higher specificity and flexibility allowing a better orientation of its multiple arms and the binding to several CD47 molecules expressed on the surface of cancer cells and CSC.

KEYWORDS

Cancer, CD47, nanobody, streptabody, CSC, aptamers.

ACKNOWLEDGEMENTS

The results of the project were achieved with support of the Ministry of Education and Science of the Russian Federation as a part of the agreement 14.604.21.0110 of the Federal Special-Purpose Programme "Research and development in the high priority development fields scientific and technological complex of Russia for 2014 - 2020".

SUMMARY

Development of high affinity molecules possessing the ability to block or modify the functional activity of receptors on the surface of cancer cells might have great

application in perspective personalized therapy of tumor diseases. It is known that most types of cancer relapse is due to resistance to chemotherapy and high proliferative activity of so-called cancer stem cell (CSC) population. This resistance is ensured by overexpression of a number of receptors on the surface of cancer cells (CD47, CD44, CD133, etc.). CD47 protein is expressed at high level on the surface of many cancer cells. CD47 interacts with SIRPa receptor which is present on macrophages resulting in phagocytosis inhibition. Thus cancer cells can escape their recognition by the host immune system. CD47-SIRPa interaction is considered as a promising target for cancer therapy. Howewer, antibodies with properties suitable for clinical application are still under development. VHH antibodies and their various multivalent forms might be promising therapeutic agents which may be represented by a new high affinity anti-CD47 VHH-antibody which has a better blocking action, smaller size and minimal toxicity. VHH-antibodies have several advantages over single-chain antibodies derived from conventional molecules of IgG such as simplicity of genetic manipulation, high expression in different systems, good solubility, high stability in a wide range of conditions and better tissue penetration due to smaller size (15-30 kDa). Antibody aCD47cl19VHH was obtained in our lab by phage display technology and leads to apoptosis of lymphoma cell line U937. Now our aim is to increase the functional affinity (avidity) of VHH fragments by tetramerization on streptavidin, following their site-specific biotinylation by the enzyme BirA. Expression vector have been constructed that enable addition of the 15 amino acid biotin acceptor domain (BAD) on aCD47cl19VHH. Different domains were cloned at the C-terminus of VHH in the following order: a semi-rigid hinge region (of 16 residues), the BAD, and a histidine tail. Monomeric form of aCD47cl19VHH-BAD were first synthesized in Escherichia coli carrying the plasmid encoding the BirA enzyme, and then purified from the cytoplasmic extracts by Ni–NTA affinity chromatography. aCD47cl19VHH-BAD has KD about 3 nM which is lower than for B6H12.2 monoclonal antibody. It will expected that streptabody form might have higher specificity and flexibility allowing a better orientation of its multiple arms and the binding to several CD47 molecules expressed on the surface of cancer cells and CSC.

ADDITIONAL INFORMATION

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Rogaev Evgeny

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Genomics of brain functions and brain pathologies

SCIENTIFIC ORGANIZATION

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KEYWORDS

Genetics, epigenetics, neuropsychiatric diseases, behavioral traits.

ACKNOWLEDGEMENTS

Supported by the Government of the Russian Federation (Project №14.B25.31.0033, Resolution No.220 Federation of April 9, 2010). The researchers of Center of Brain Neurobiology and neurogenetics contributed to the results (presented, in part, as the separate poster abstracts). We thank Dr. Trut L.N, Dr. Markel A.L., Dr. Trapezov O.V. for the material and discussions. Dr. Kolchanov N.A. for general support.

SUMMARY

We applied new generation sequencing (NGS) technologies to track the genetic and epigenetic alterations underlying common and rare neuropsychiatric diseases and behavioral traits. In this presentation the methodologies for the whole genome sequencing and epigenome or transcriptome analysis will be summarized for (i) identification of mutant gene linked to impairment of human-specific phenotype (bipedal locomotion, intellect and speech) inherited as monogenic trait in human pedigree ; (ii) tracking open chromatin alterations in cortical neurons in cohort of schizophrenic patients versus controls; (iii) identification of genetic variants and gene neuro-net pathways in Alzheimer's disease; (iii) identification of genetic variations in behavioral farm-lab animal models selected for tame and aggressive behavior.

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Y-tools: a novel toolkit for analysis of antibody repertoires using immunosequencing data

SCIENTIFIC ORGANIZATION

Saint Petersburg State University

ABSTRACT

The analysis of circulating antibodies is a fundamental problem in immunoinformatics. Antibodies are not encoded in germline but are diversified by gene recombination and mutations. These processes complicate reconstruction of the original repertoire from sequencing data. On the other hand, antibody repertoire is custom for each individual that results in a lack of gold standard test datasets. To address these challenges, we are developing a toolkit for immunoinformatics analysis including repertoire construction algorithm, tools for clonal and quality assessment analysis.

KEYWORDS

Immunoinformatics, personal medicine, immunology, antibody repertoire.

SUMMARY

Reconstruction and analysis of antibody repertoire is an important part of various immunological studies. While modern biotechnologies allow one to perform deep and full length scan of circulating antibodies using immunosequencing and mass spectrometry, there is no gold standard toolkit for their analysis. Here we present a novel multipurpose toolkit for construction and investigation of adaptive immune repertoires using immunosequencing and mass spectra data. It includes IgRepertoireConstructor [1], an algorithm for antibody repertoire construction and immunoproteogenomics analysis; AntEvolo, an algorithm for construction of clonal trees and evolutionary analysis of antibody repertoires; aimQUAST [2], a quality assessment tool for adaptive immune repertoires; and IgSimulator [3], a versatile simulator of antibody repertoire. IgRepertoireConstructor, IgSimulator and aimQUAST are freely available at Github. AntEvolo to be released in fall 2016.

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Gene network of interaction between Alzheimer's disease and lipid metabolism reconstructed by ANDSystem

SCIENTIFIC ORGANIZATION

Institute of Cytology and Genetics of the Siberian Branch of the Russian Academy of Sciences

ABSTRACT

Nowadays it becomes obvious that Alzheimer's disease (AD) is very complex. Recently it was shown that lipid metabolism (LM) is involved in the progression of Alzheimer's disease. The mechanisms linking lipid metabolism and Alzheimer disease are still not well understood. The goal of this study was to reconstruct and analyze gene network linking lipid metabolism and Alzheimer disease. This knowledge may give a deeper understanding of molecular-genetic basis of Alzheimer disease.

KEYWORDS

Gene network, Alzheimer's disease, lipid metabolism, ANDSystem.

ACKNOWLEDGEMENTS

This work has been done by the finance support of the Government of the Russian (Project №14.B25.31.0033, Resolution No.220 Federation of April 9, 2010).

SUMMARY

Motivation and Aim: Alzheimer's disease (AD) is a complex neurodegenerative disease characterized by β-amyloid plaque formation in human brain. The formation of amyloid plaques is modulated by cellular cholesterol. The cholesterol level in brain is increased during the AD progression (Hannaoui et al., 2014). Nevertheless the mechanisms linking the lipid metabolism and AD are not yet well understood. The goal of this study was to reconstruct and analyze gene network connecting the lipid metabolism and AD. This study may identify novel molecular pathway elements for AD and can contribute to improvement of existing AD therapy approaches.

Materials and methods: Gene list associated with lipid metabolism was formed based on the information from scientific publications, Coremine system (makes statistical assessment for terms co-occurrence in publications) and Gene Ontology annotation. List of genes associated with Alzheimer's disease was extracted from GWAS Catalog, OMIM, GeneCards databases, MeShops and CoreMine systems and ANDSystem (Ivanisenko et al., 2015). Gene networks reconstruction was performed by ANDSystem that utilize automated literature mining approach (text-mining). Information on drug targets was extracted from DrugBank database. Gene Ontology enrichment analysis was performed by DAVID. Betweenness centrality of a protein in a network was calculated by R package igraph. Statistical significance difference of distributions was assessed by t-test and Mann–Whitney U test implemented in Python library SciPy.

Results:

Reconstruction of gene network associated with lipid metabolism.

List of 1451 genes associated with lipid metabolism was obtained by manual analysis of scientific publications and automated methods from Coremine and Gene Ontology annotation and used for gene network reconstruction by ANDSystem. In the reconstructed gene network associated with lipid metabolism 1029 proteins were connected by 7734 interactions.

Reconstruction of gene network associated with Alzheimer's disease.

List of 884 genes associated with Alzheimer's disease was extracted from databases (GWAS Catalog, OMIM, GeneCards), MeShops and CoreMine systems and ANDSystem. In the reconstructed gene network associated with AD 595 proteins were connected by 6626 interactions.

Reconstruction and analysis of gene networks describing interaction between lipid metabolism and Alzheimer disease.

We found that 150 proteins are common for AD and LM gene networks. Among them 100 proteins are known drug targets. It is reasonable to speculate that intake of such drugs could potentially cause adverse effects related to AD or vice versa can imply a potential therapeutic molecule. For example, pravastatin has a neuroprotective effect (Corrao et al., 2013).

To investigate if genes associated with Alzheimer's disease are core in the lipid metabolism network we compared the distributions of betweenness centrality of genes associated with AD and LM simultaneously and genes associated with LM. Betweenness centrality of a node in a network is equal to the number of shortest paths from all vertices to all other nodes that pass through that node. A node with high betweenness centrality has a large influence on the network. Comparing the betweenness centrality distribution for proteins associated with AD and LM with the same distribution built on LM proteins demonstrated significant differences from each other ($p<0.0001$). The average numbers of betweenness centrality for proteins associated with AD and LM was 1479 while for all proteins associated with LM it was only 523. Thus we can speculate that genes associated with Alzheimer's disease play essential role in lipid metabolism network. Several studies indicated that cholesterol metabolism may contribute to AD (Hannaoui et al., 2014). We found that the "cholesterol metabolic process" cluster is statistically significant enriched by proteins associated with AD (p-value<0.0001).

There is evidence that some diseases associated with alterations of lipid metabolism, such as obesity, weight loss (Leboucher et al., 2013), atherosclerosis

(Ismailov, 2013), dyslipidemias and diabetes mellitus (Akomolafe et al., 2006) can influence AD pathogenesis. Statistical analysis showed that these diseases have more common genes with AD than it could be expected ($p<0.0001$).

This work has been done by the finance support of the Government of the Russian (Project №14.B25.31.0033, Resolution No.220 Federation of April 9, 2010).

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ADDITIONAL INFORMATION

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Chromosome structure

SCIENTIFIC ORGANIZATION

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ABSTRACT

The chromosomes of multicellular animals are organized into a series of topologically independent looped domains. This domain organization is critical for the proper utilization and propagation of the genetic information encoded by the chromosome. A special set of architectural elements, called boundaries or insulators, are responsible for both subdividing the chromatin fiber into discrete domains, and determining the topological organization of these domains.

KEYWORDS

Chromosomes, loop topology, boundary elements/insulators.

ACKNOWLEDGEMENTS

Research supported by grants from the Russian Federation Ministry of Education and Science (14.B25.31.0022) and the National Institutes of Health, USA (RO1-GM043432).

SUMMARY

The highly regular and reproducible physical organization of chromosomes in multicellular eukaryotes was first recognized more than a century ago in cytological

studies on the lampbrush chromosomes that are found in oocytes arrested at the diplotene phase of meiosis I. At this stage, homologous chromosomes are paired. The two homologs display a similar and reproducible architecture. It consists of a series of loops emanating from the main axis of the chromosome that are arranged in pairs, one from each homolog. In between the loops are regions of more compacted chromatin. We now know that the chromosome architecture of oocyte lampbrush chromosomes is not restricted to these highly specialized chromosomes, but instead is a characteristic feature of chromosomes in multicellular eukaryotes. Like the oocyte lampbrush chromosomes, chromosomes of somatic cells are subdivided into a series of topologically independent looped domains. Underlying this architectural organization are special DNA sequences called boundary elements or insulators. Our research is aimed at understanding how boundary elements subdivide the chromosome into topologically independent domains, and elucidating the genetic and regulatory consequences of this organization.

ADDITIONAL INFORMATION

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Seamus Martin
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Leading Scientist

Identification of antagonists of psoriasis-associated IL-36 cytokine activation

SCIENTIFIC ORGANIZATION

Saint Petersburg Institute of Technology

ABSTRACT

IL-36α, IL-36β and IL-36γ, have been implicated as key initiators of psoriatic-type skin inflammation. IL-36 cytokines are expressed as inactive precursors and require proteolytic processing for activation. We have developed a panel of peptide-based inhibitors of cathepsin G and elastase, based on optimal cleavage motifs, which can antagonize activation of all three IL-36 family members by the latter proteases. Inhibitors of neutrophil-derived proteases, as reported herein, may have therapeutic utility through blocking activation of IL-36 family cytokines in psoriasis.

KEYWORDS

Inflammation, proteases, proteolysis, neutrophils.

ADDITIONAL INFORMATION

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Epigenetic study of early childhood

SCIENTIFIC ORGANIZATION

Saint-Petersburg State University

ABSTRACT

The thesis considers the issue of the influence of early experience on both physical and mental health. The notion of epigenome is discussed in the context of deprivation and the review of previous studies in animals and human of this issue is provided. At the end of the thesis a description of the current research of the problem is given, which is carried out under the governmenntal grant of the RF «Impact of early deprivation on bio-behavioral indicators of child development» at the Laboratory of Translational Sciences of Early Childhood, SPSU.

KEYWORDS

Epigenetics, deprivation, early life experience.

SUMMARY

Due to the rapid development of scientific disciplines that arose at the intersection of biology and psychology (psychophysiology, neuropsychology, psychogenetics), the use of biological methods in psychological studies is increasingly actual.

One of the promising interdisciplinary areas in terms of research of deprivation impact on human development is behavioral epigenetics. This new psychogenetic branch studies the role of epigenetic mechanisms in the formation of behavioral phenotype under the influence of environmental factors. Currently a special research interest is focused on the transformations of the epigenome (changes in gene expression regulation mechanisms) associated with early adverse external conditions. These transformations are supposed to result in long-term consequences for the physical and mental development and health of the child.

One of the major epigenetic mechanisms of regulation of gene activity is DNA methylation – a process consisting in attachment of a methyl group (CH3) to cytosine, which eventually leads to suppression of expression of the corresponding gene. The set of methylated regions of the genome constitutes structures specific to different types of cells – DNA methylation patterns (Strathdee and Brown, 2002).

The studies of SD Suomi, HF Harlow, SD Kimball, D. Liu, DK Day, carried out on animals, revealed that the early separation from mother has negative effects on the offspring`s behavior and health (Suomi et al., 1971; Liu et al., 2000). Researchers D. Chiccetti, MR Gunnar, M. Dozier, KO Ladd received data confirming the negative impact of early adverse experience on human development (Cicchetti, 2002; Ladd et al., 2000). Furthermore, the study of mental and physical health of children from social institutions conducted by TG O `Conner, MR Gunnar H. Fox, C. Nelson, Ch Zeanah allowed to draw conclusions about the difficulties in the development of emotional, cognitive, motor and communicative spheres of these children (O'Connor et al., 2000; Zeanah et al., 2003).

Negative childhood experience is associated with the risk of a wide range of diseases and behavioral problems in later adulthood (Felliti et al., 1998; Shonkoff et al., 2009). Epidemiological studies show that a range of diseases, such as cardiovascular disease, diabetes, obesity, depression, substance abuse, premature aging and others have their determinants in the early stages of development (Harkonmaki, 2007; Shonkoff et al., 2009; Felliti et al., 1998; Coelho et al., 2014), and a number of them is associated with early deprivation (Kreppner et al., 2007).

Despite the relative "youth" of behavioral epigenetics in general, and studies of epigenetic response to the conditions of early deprivation, in particular, this area is actively being developed by foreign scientists during the last decade. It is reflected in numerous foreign literature reviews in the area (Hoffmann & Spengler, 2014; Lutz & Turecki, 2013; Szyf, 2013). In Russia this area of research remains largely unexplored.

Evidence provided both by animal and human studies support the hypothesis that maternal care has a huge impact on the phenotype of progeny, and that this effect is probably mediated by changes in gene expression and epigenetic regulation of

its systems. Consequently, the understanding of the mechanisms involved in the occurrence of the phenomena discussed above, requires the study of "epigenetic response" on a factor of deprivation and its role in shaping the phenotype, in the context of the features of the child's development and long-term effects of deprivation conditions on mental and physical health.

Epigenetics is the science that deals with the study of gene expression changes caused by mechanisms that do not affect the DNA sequence. Epigenetic mechanisms are numerous and complex, with basic one represented by RNA interference, chromatin reconstruction, histone modification and DNA methylation (Turner, 2001). However, we will focus on discussing the DNA methylation. DNA sequence has some specific sites where the methyl group can attach to cytosine using enzymatic reactions. Such sites are usually located within the regulatory regions of gene, near the promoter preceding the initial transcription site. Thus, methylation is a covalent modification of DNA by attachment of a methyl group (CH3) to cytosine contained in the dinucleotide sequence cytosine-guanine (CpG), which leads to suppression of gene activity. At the functional level methylation restricts access of transcription factors and RNA polymerase to the DNA. The link between cytosine and methyl group is very strong, which results in stable, although potentially reversible changes in expression. Patterns of DNA methylation are saved during cell division and are transferred, thus, to the daughter cells, and it is through this mechanism that cell differentiation occurs (Turner, 2001). An important direction is behavioral epigenetics – young psychogenetic area, which aim is to study the patterns of environmental influence on the epigenome and the phenotypic manifestations of such interaction, which include, in particular, the emergence of various diseases, certain forms of behavior and trajectories of mental development.

The molecular basis of long-term effects of maternal deprivation on progeny phenotype was first demonstrated in a series of experiments with rats conducted by Moshe Zif and Michael Meaney. The researchers observed the behavior of rats exhibiting high and low level of care to their offspring, and then examined the differences in mRNA hippocampal glucocorticoid receptors in the latter (Weaver et al., 2004). At the phenotypic level rats reared by caring mother, showed blunted reaction to a stressful situation from the hypothalamic-pituitary-adrenal axis, and also showed a lower incidence of anxious behavior (Meaney et al., 1996; Liu et al., 1997). It was noted that a high level of caring behavior in mothers changed epigenome of progeny rats at promoters of genes encoding the glucocorticoid receptors of the hippocampus. The researchers found differences in DNA methylation in pups reared by caring mothers, compared with the offspring of inattentive mothers. The level of glucocorticoid receptors in the hippocampus regulates HPA axis response to stress on the feedback principle: a high level of activity of mRNA glucocorticoid receptor corresponds with poor response to stress (Jacobson and Sapolsky, 1991).

There are also studies concerning the possibility of transferring the effects of early experience through the generations. For example, T. Franklin on the basis of observations over mice, subjected to prolonged and unexpected separation from the mother during 14 days after birth, succeeded to show that prolonged separation entails manifestation of behavior peculiar to depression at an older age and changes their behavioral reactions towards negative and dangerous environmental factors. Such behavioral changes appeared later in progeny of mice who had experienced maternal separation, in spite of the fact that they grew under normal conditions. Long and unpredictable separation from the mother has also changed the profile of DNA methylation in promoters of several candidate genes of germline in separated males. Similar changes in DNA methylation associated with altered expression of genes have been identified in the brains of their offspring. Described data illustrate the vast deleterious effects of stress on early development and behavioral responses, transmitted across generations through the regulation of DNA methylation. Mouse model presented here reproduces the multiple effects of early stress on behavior and reflects the unique and unprecedented model of inherited behavioral disorders due to early stress. (Franklin et al., 2010).

There are also attempts to study the applicability to human of the thesis, developed on the basis of studies in animal models. Recently there were described studies on genome-wide changes in DNA methylation in peripheral tissues after the experience of interaction with adverse early environment. In the first study, an attempt was made to trace the link between DNA methylation in blood and evidence of early abuse, post-traumatic stress disorder and exposure to stress (Smith et al., 2011). While differential methylation in gene 1 and 5 associated with PTSD and stress, there were found no statistically significant results on the experience of early

violence. In another study in the saliva of children who have experienced abuse at early age there were found 2600 CpG sites, which methylation level was different from the level of methylation in children, who have never faced with violence and had no mental illness (Yang et al., 2013). Along with the previous findings, these studies suggest that the violence faced in early childhood, and the related stressor experience have profound genome-wide epigenetic consequences for peripheral tissues.

Of particular interest to us is the study conducted recently by O. Naumova and colleagues, which checks for a connection between the experience of deprivation conditions in early childhood and changes in gene expression (Naumova et al., 2012). The aim of this study was to compare the genome methylation patterns in children-orphans and children from biological families. Comparative analysis of methylation of two groups of children identified about 800 differently methylated gene and showed that the most important intergroup difference was the increased level of methylation of the genomes of children in orphanages, as compared with children living in biological families. Thus, there were many high-methylated genes in children from these institutions, which play an important role in controlling the immune response and cell signaling systems as well as in the development and functioning of the brain.

Our interdisciplinary research project called «Impact of early deprivation on bio-behavioral indicators of child development» represents another attempt to study change of the epigenome in early childhood, in the context of various and dynamic social environments – institutional care (IC), foster care (FC) and typical family environment (typically developing, TD). The research is a cross-sectional study of the complex of behavioral, neurophysiological and epigenetic indicators of children.

Our hypothesis is that institutional care may cause systematic changes in the DNA-methylation profiles of children, that in turn may exert an impact on biological and behavioral levels of the children`s development. These alterations may be neutralized or reversed with changes in care, such as the children's placement into foster families.

The study involves a sample of children with Down syndrome, which gives an opportunity to examine the character of epigenetic perversions in their genomes. We hypothesize that analysis of data collected will provide new evidence on global alterations in the epigenome related to trisomy, and will allow to identify some features of epigenetic patterns associated with cognitive impairments in DS children.

We suggest that our unique data will provide significant results of epigenome-wide association with behavioral phenotypes on early stages of the development.

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Defects in antiviral signaling as factors promoting viral oncolysis

SCIENTIFIC ORGANIZATION

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ABSTRACT

Viral infection leads to the activation of multiple innate antiviral cellular pathways. Cytokines of the type I IFN system possess a wide range of biological activities: they are able to block replication of some viruses and to induce growth inhibitory and/or apoptotic cell signals. Many cancer cells have been demonstrated to possess defects in antiviral signaling pathways that allow them to resist IFN-induced growth-inhibitory and apoptotic signals.

KEYWORDS

Cancer, oncolytic virus, interferon.

SUMMARY

Although interferon-non-responsive cancer cells may have acquired a growth/survival advantage over other cells, they are more susceptible to viral infections, therefore, they are probably more sensitive to oncolytic virotherapy.

Our aim was to analyze correlation between defects in antiviral signaling pathway of different cancer cell lines and their susceptibility to oncolytic viruses. We identified ability of cancer cells to respond to treatment with interferon. It was shown that among different groups of cancer exist IFN sensitive and completely resistant cancer cell lines. Then we assessed ability of cancer cells to produce IFN in response to induction with virus. There was also a significant difference between amounts of secreted IFN: some lines exhibited production of IFN on comparable to normal cells level, while others had undetectably low, if any, quantity. We also established correlation between identified defects and susceptibility of cancer cells to oncolytic viruses.

ADDITIONAL INFORMATION

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Junior scientist

Development of intrinsic optical signal in somatosensory cortex of neonatal rat

SCIENTIFIC ORGANIZATION

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ABSTRACT

Intrinsic optical signal (IOS) associated with active brain tissue is promising yet challenging functional imaging technique due to very low SNR values. We showed that, in contrast to fMRI, IOS is applicable for imaging of somatosensory cortex of neonatal rats since P3 (P0 for birth). Our data suggest that in neonatal rats IOS and fMRI have different origins.

KEYWORDS

Intrinsic optical signal, ontogeny, somatosensory cortex, barrel.

ACKNOWLEDGEMENTS

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SUMMARY

Functional imaging is a perspective and promising way to study how the brain works. Modern imaging techniques are widely used both in clinic and fundamental

science. One of the imaging techniques is based on registration of intrinsic optical signal (IOS), which is considered to be a functional analogue to the BOLD fMRI, i. e. both techniques are registering hemodynamic responses in active region. However we have already shown a presence of IOS in neonatal rats, whereas BOLD fMRI response appears significantly later in development, thus raising a question whether both techniques use similar parameters of active tissue. To answer it we focused on detection and analysis of IOS in vivo in anesthetized newborn rats using whisker stimulation during first three weeks after birth. To improve signal-noise ratio of IOS we used video preprocessing (light and motion corrections, spatial and temporal filtering), which allowed us to observe IOS presence since P3 (P0 corresponds to the day of birth). Analysis of developmental profile revealed significant correlation between optimal stimulation and animal age: the older the animal the more frequent stimulation it supports. The bell shape of IOS dependence on age with maximum at P9-P10 was equally found. We performed simultaneous IOS and EEG recording from the principal barrel and established a relationship between IOS and electrical neuronal activity. Our findings suggest that in neonatal rats IOS and fMRI have different origins, thus making IOS suitable for brain imaging early in development.

Sivova Irina
Student

Impact of interferon system on Paramyxovirus-mediated oncolysis

SCIENTIFIC ORGANIZATION

Engelhardt institute of molecular biology of the Russian Academy of Sciences

ABSTRACT

Oncolytic virotherapy is a new progressive approach of anticancer therapy. Oncolytic viruses naturally replicate preferentially in cancer cells leading to killing tumor cells without harming normal tissue. Mitochondrial antiviral-signaling protein (MAVS), is an important key molecule involved in host defense and promotes a signal for producing type I IFN. Here we demonstrated the correlation between sensitivity cancer cell line to paramyxoviruses action and cancer cells MAVS expression level.

KEYWORDS

Oncolytic virus, cancer therapy.

ACKNOWLEDGEMENTS

Sidorenko A.S., Tereshkova A.V.

SUMMARY

Oncolytic virotherapy is a new progressive approach of anticancer therapy. Oncolytic viruses naturally replicate preferentially in cancer cells leading to killing tumor cells without harming normal tissue. Paramyxoviruses are thought to be an advanced oncolytic virus family which also can stimulate immune system effectively. Interactions between innate and adaptive immune cells and signaling factors (i.e., cytokines and chemokines), often involved in virus infections, play a large role in antitumor immunity.

Mitochondrial antiviral-signaling protein (MAVS), also called IPS-1/VISA/Cardif, is an important key molecule involved in host defense and promotes a signal for producing type I IFN. Here we demonstrated the correlation between sensitivity cancer cell line to paramyxoviruses action and cancer cells MAVS expression level.

We tested the wide panel of cancer cell lines to define its sensitivity to paramyxovirus action. We established that cancer cell lines possess different sensitivity to Sendai viruses which is invert correlated with basic level of MAVS expression. Moreover, silencing of the endogenous MAVS expression by RNAi lead to significant increasing cancer cells sensitivity to paramyxovirus action.

Studitsky Vasily
Doctor of Science

Gerasimova Nadezhda
Junior Researcher

SCIENTIFIC ORGANIZATION

Lomonosov Moscow State University

Chromatin Transcription: Epigenetics, Cancer & Aging

ABSTRACT

Human genome is compacted by histone proteins into chromatin that significantly limits DNA accessibility, providing a barrier that participates in regulation of RNA synthesis and other processes in the cell. Misregulation of these processes causes various human diseases including cancer and early aging. Our laboratory studies the molecular mechanisms involved in regulation of gene expression in chromatin and their misregulation during cancer development and aging.

KEYWORDS

Chromatin, epigenetics, cancer, aging, transcription, nucleosome, gene regulation.

ACKNOWLEDGEMENTS

This work was supported by the grant № 11.G34.31.0009 in Russian Federation Government Ordinance № 220, the Ministry of Education and Science of the Russian Federation (Contract 14.512.11.0028), the Federal Target Program "Research and developments in the priority directions of the scientific-technological complex of the Russian Federation for 2014–2020" (Agreement of the Ministry of Education of the Russian Federation No 14.604.21.0063, RFMEFI60414X0063), the Program of the Presidium of the Russian Academy of Sciences "Basic Research for the Development of Biomedical Technologies" (FIMT2014011), and the Russian Science Foundation (RSF 14-24-00031).

SUMMARY

Development and functioning of living organisms critically depends on proper gene expression. Regulation of genes involves a very complicated and fine-tuned interplay between specific nucleotide sequences, protein factors and dynamic changes in the spatial organization of the genome. In higher organisms regulation of gene expression occurs primarily at the step of transcription.

The majority of eukaryotic genes are transcribed by RNA polymerase II (Pol II). In the nucleus of eukaryotic cells DNA is organized in chromatin – tightly compacted DNA-protein complexes (nucleosomes) forming repeating units of genome organization on every ~200-bp region of the genome. Pol II meets these DNA-protein complexes during transcription, and they are likely targets for gene regulation at the level of transcript elongation. Nucleosomes present a high polar barrier for the enzyme *in vitro*[1], but various protein factors allow efficient transcription through chromatin and facilitate histone survival[2,3]. Overall, the Pol II-specific mechanism of transcription through chromatin is likely used for maintenance of chromatin structure and the "histone code" that is particularly important during genomic transcription. The key features of Pol II–nucleosome encounter are conserved from yeast to human, highlighting the importance of this mechanism for the cell.

In our studies we have established a "minimal", highly purified and efficient experimental system maintaining single- and multiple-round transcription through various defined mono- and polynucleosomes by yeast and human RNA polymerase II faithfully recapitulating numerous features of transcribed chromatin described in vivo and allowing their molecular analysis *in vitro*[4].

Recent structural analysis of intermediates formed during transcription through chromatin allowed us to propose the mechanisms of nucleosomal barrier formation and nucleosome survival during transcription[5,6]. It indicated that both DNA–histone interactions and Pol II backtracking contribute to formation of the high nucleosomal barrier to transcription. Nucleosome survival during transcription likely occurs through allosterically stabilized histone–histone interactions. The data reveal the importance of intranucleosomal DNA–protein and protein–protein interactions during conformational changes in the nucleosome structure on transcription. The proposed mechanism suggests that the high nucleosomal barrier to Pol II participates in regulation of gene expression in eukaryotes and explains the remarkable efficiency of nucleosome survival during transcription, important for maintenance of epigenetic and regulatory histone modifications. Our recent structural analysis of other inter-

mediates formed during transcription through chromatin will be presented.

Nucleosome structure and dynamics significantly affect DNA accessibility to other regulatory and effector proteins, for example, to DNA repair systems. In our studies we have shown that transcription through chromatin is accompanied by formation of small intranucleosomal DNA loops. Pol II captured within a small loop drives accumulation of DNA supercoiling, facilitating further transcription. DNA breaks relieve supercoiling and induce Pol II arrest, allowing detection of DNA damages hidden in chromatin structure[7]. Our recent studies of this novel chromatin-targeted mechanism of DNA repair will be presented.

FACT (facilitates chromatin transcription) is an essential and highly conserved histone chaperone that assists nucleosome assembly and disassembly, and plays an important role in cell differentiation and cancer development. Our previous studies have suggested that human FACT (hFACT) facilitates transcription through chromatin and promotes nucleosome recovery *in vitro*[3]. FACT also increases the accessibility of nucleosomal DNA to regulatory proteins, but the mechanism and extent of this nucleosome reorganization are unknown. Our recent studies using single particle FRET microscopy revealed a dramatic and reversible uncoiling of nucleosomal DNA by FACT. This FACT-dependent nucleosome unfolding modulates the accessibility of nucleosomal DNA, and plays an important function of in vivo. Similar mechanisms are likely used during various other processes involving DNA, including DNA replication and ATP-dependent chromatin remodeling.

Our most recent studies are conducted using a combination of molecular genetics, genomics, biochemical, single-particle, structural and computational modeling approaches and are focused on the mechanisms of transcription through chromatin and action of various elongation factors and histone chaperones (hFACT and hPARP1, both are involved in cancer development and aging and are important targets for anti-cancer drugs) facilitating histone survival during this process. The developed experimental models allow construction of test systems for new anti-cancer drug screening and further analysis of the complicated mechanisms of regulation of gene expression.

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ADDITIONAL INFORMATION

Co-authors of the presentation: Maria E. Valieva, Nadezhda S. Gerasimova, Grigori A. Armeev, Kseniya S. Kudryashova, Alexey K. Shaytan, Dmitry V. Nikitin, Oleg V. Chertkov, Olga I. Kulaeva, Olesya I. Volokh, Olga S. Sokolova, Alexey V. Feofanov, Mikhail P. Kirpichnikov, Vasily M. Studitsky.

Suchkov Dmitrii
Junior Researcher

L6 modulates cortical activity in the neonatal rat pups

SCIENTIFIC ORGANIZATION

Kazan (Volga region) Federal University

ABSTRACT

Barrel cortex contains a topographic map of the facial whiskers formed by the functionally united groups of neurons of layer 4 that forms visually detected structures - barrels. Recently it was shown that among thalamic excitatory inputs barrel's layer 4 (L4) has also inhibitory inputs from infragranular layer 6 (L6). We have found that inhibitory effect of L6 on L4 is established starting from the first postnatal week. Emergence of the L6 evoked inhibition during critical period of the barrel cortex development suggests that L6 possibly is involved in the formation of cortical maps.

KEYWORDS

Rat, cortex, barrel, critical period, layer 4, layer 6.

ACKNOWLEDGEMENTS

Sintsov M.*, Khazipov R.** and Minlebaev M.** * IAL "Developmental neurobiology", Kazan, **INSERM, Marseille.

SUMMARY

The barrel cortex in rodents is responsible for the contact of the animal with the external world using vibrissa on the whisker pad of the animal. It contains a topographic map of the facial whiskers formed by the functionally united groups of neurons of layer 4 that forms visually detected structures - barrels, where each barrel is tuned to a corresponding whisker. Recently it was shown that among thalamic excitatory inputs barrel's layer 4 (L4) has also inhibitory inputs from infragranular layer 6 (L6). Recently group of Scanziani demonstrated that L6 modulates cortical activity through an inhibition and identifies the neurons that are able to regulate the strength of cortical responses throughout cortical depth. However, the question remains what is the role of this modulation and when this modulation of the L4 activity by L6 emerges. In our research we have found that inhibitory effect of L6 on L4 is established starting from the first postnatal week. Activation of the L6 neurons following early gamma oscillation (EGO) in layer 4 strongly modified it that resulted in disappearance of the EGO cycles. Emergence of the L6 evoked inhibition during critical period of the barrel cortex development suggests that L6 possibly is involved in the formation of cortical maps.

Terekhin Vladimir
PhD
Senior scientists

Mesoporous microcapsules based on polystyrol SiO2 core/shell nanoparticles: synthesis and functional carrier's properties

SCIENTIFIC ORGANIZATION

Moscow Engineering Physics Institute

ABSTRACT

The controlled release of drugs from an matrix has become important for therapeutic systems. Among a variety of drug delivery systems, mesoporous silica capsules have several advantages for use in the delivery of drugs. These materials have large surface areas and porous interiors that can be used as reservoirs for storing the drug. A novel method for preparation of hollow silica capsules was developed. The silica capsules with tuned wall thickness were obtained and used as drug carriers for amoxicillin loading and for investigation amoxicillin in vitro release.

KEYWORDS

Core/ shell composite particles, mesoporous SiO2 capsule, drug release.

ACKNOWLEDGEMENTS

This study was supported by the Federal Targeted Program for Research and Development of the Ministry of Education and Science of Russian Federation (Grant 14.578.21.0054, Contract No. RFMEFI57814X0054).

SUMMARY

Inorganic hollow microspheres are used in various fields of research and technology, e.g., as containers for drugs [1–4], absorbents [5], and catalysts [6]. An effective technique for obtaining such capsules is the removal of the core from organic core/inorganic shell composite particles (CPs). Polystyrene (PS) core/SiO2 shell particles are apparently the most widely used CPs. The morphology of the capsules obtained by this method is determined by the structure of the original CPs.

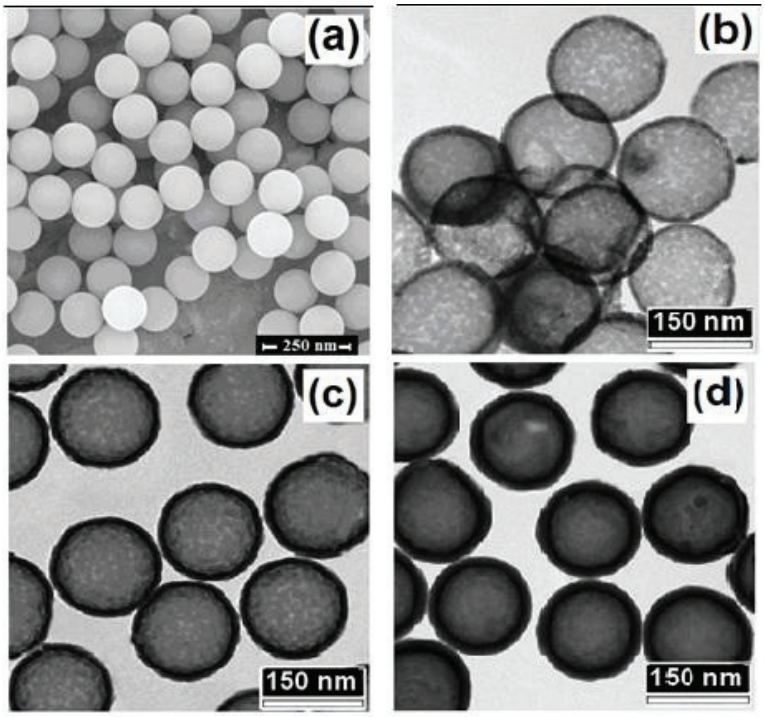

Fig. 1. (a) A scanning electron microscopic image of the synthesized polystyrene particles. (b, c, d) Microphotographs of SiO_2 shells obtained after thermal treatment of the composite particles synthesized at tetraethyl orthosilicate concentrations of (b) 0.05, (c) 0.2, and (d) 0.4 M.

In this study, Stober's method was used to synthesize PS core/SiO2 shell CPs. The dependences of the SiO2 shell structural parameters, including the width, roughness, uniformity, continuity, and porosity, on the conditions of its formation (pH, tetraethyl orthosilicate (TEOS) concentration, reaction time, and the concentration and molecular weight of polyvinylpyrrolidone (PVP)) were determined. It has been demonstrated that variation of these conditions allows SiO2 shells with widths from ~4 to 17 nm and different morphologies to be formed on PS particles (Fig. 1).

The PVP molecules preliminarily absorbed onto the surface of the PS particles have been shown to be incorporated into the SiO_2 shell in the course of its formation, which results in pores ~3 nm in diameter. By varying the PVP concentration in the reaction mixture, one can change the number of pores and the specific areas of the surfaces of CPs and SiO_2 capsules obtained from them within a wide range.

It has been demonstrated that the resultant mesoporous SiO_2 capsules can be used as containers for drugs (here, amoxicillin was used as a model drug). The kinetics of the release of amoxicillin from the loaded capsules was studied under the conditions

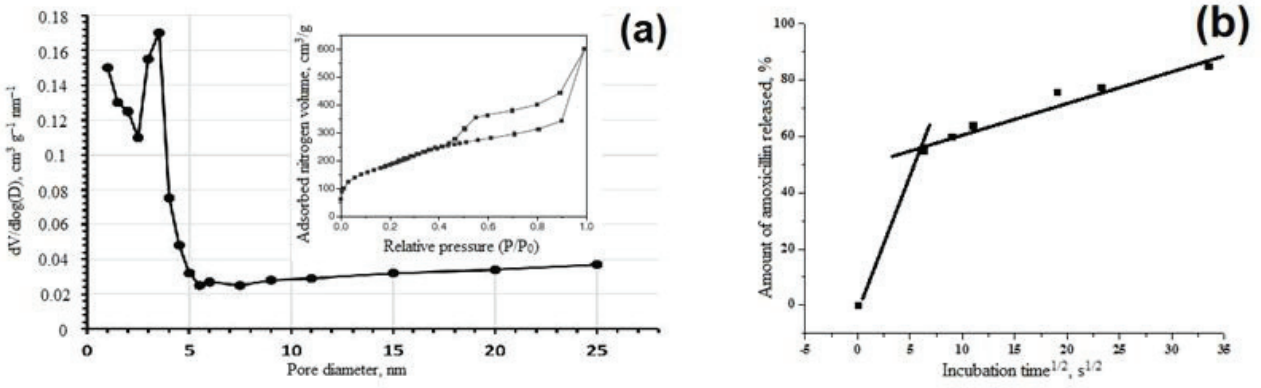

Fig. 2. (a) The size distribution of pores in SiO_2 shells obtained by thermal treatment of the composite particles at 400°C. The inset shows a typical adsorption–desorption isotherm of a sample of the SiO_2 capsules formed as a result of thermal treatment of the composite particles at 400°C. (b) The dependence of the amoxicillin concentration on the time of incubation of loaded SiO_2 capsules in a medium simulating a human biological fluid.

close to physiological ones (the capsules were incubated in a medium simulating a human biological fluid). The amoxicillin release has been proved to be a diffusion-controlled process, as evidenced by the pattern of dependence of the amount of the drug released on the square root of the incubation time, which was close to linear (Fig. 2). The deviation from a strictly linear dependence is explained by variation of the diffusion coefficients at different stages of the amoxicillin release.

This study was supported by the Federal Targeted Program for Research and Development of the Ministry of Education and Science of Russian Federation (Grant 14.578.21.0054, Contract No. RFMEFI57814X0054).

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Tereshkova Alesya
Graduate Researcher

Testing oncolytic activity of human enteroviruses against glioblastoma-initiating cancer stem cells

SCIENTIFIC ORGANIZATION

Engelhardt Institute of Molecular Biology of the Russian Academy of Sciences

ABSTRACT

Glioblastomas (GBMs) are highly lethal primary brain tumors. GBMs are extremely resistant to conventional radiation and chemotherapies. A highly tumorigenic subpopulation of cancer cells, the GBM stem cells (GSCs) is the major cause of resistance to radio- and chemotherapy. Oncolityc viruses (OV) are considered as perspective agents for anticancer therapy. The OVs are believed to be capable of overcoming the problem of cancer stem cells resistance by efficiently targeting GSCs. In this study we tested oncolytic effects mediated by some strains of human enteroviruses.

KEYWORDS

Oncolytic viruses, cancer, cancer stem cells.

ACKNOWLEDGEMENTS

Sidorenko A.S., Morozov D.A.

SUMMARY

Glioblastomas (GBMs) are highly lethal primary brain tumors. GBMs are extremely resistant to conventional radiation and chemotherapies. A highly tumorigenic subpopulation of cancer cells, the GBM stem cells (GSCs) is the major cause of resistance to radio- and chemotherapy.

Oncolityc viruses (OV) are considered as perspective agents for anticancer therapy. OVs are capable of selective replication and killing of cancer cells by spreading through the tumor mass, without damaging normal tissue. The OVs are believed to be capable of overcoming the problem of cancer stem cells resistance by efficiently targeting GSCs. In this study we tested oncolytic effects mediated by some strains of human enteroviruses.

We analyzed tumor cells from primary and model glioblastomas cell line that had been cultured in a medium promoting the growth of CSCs. To estimate cancer stem cells level in patient-derived glioblastoma cell lines we used lentiviral-based report-

er system that allows direct visualization of CSCs based on functional properties. We also measured cancer stem cell count in established lines by the ALDEFLUOR assay. Increased aldehyde dehydrogenase 1A1 (ALDH1A1) activity has been found in the stem cell populations of leukemia and some solid tumors. We found an efficient killing of glioblastoma CSCs after treatment with some strains of oncolytic enteroviruses.

Tsvelaya Valeriya
Student
Engineer

Excitation of wave propagation on self-organized monolayers, formed by cardiomyocytes with pathological prolonged QT-interval

SCIENTIFIC ORGANIZATION
MIPT

ABSTRACT

Prolonged QT-interval is the important symptom of many cardiovascular diseases. Two iPSC lines reprogrammed from patient with and without pathological QT-interval, was differentiated to cardiomyocytes. Self-organization of cardio tissue culture with electro-mechanical syncytium was formed already on the 15th day after differentiation. With optical mapping and Patch Clamp methods, we measured characteristics of new cells.

KEYWORDS

QT-interval, optical mapping, iPSC, self-organised tissue

SUMMARY

Prolonged QT-interval is one of the main reasons to assign a person to the risk group of cardiovascular disease. Elongation of the QT-interval may be caused by several acquired pathologies or specific mutations. In our work, we used human induced pluripotent cells of two lines: if-31, which are reprogrammed cells from a patient with the prolonged QT-interval, as well as a control line isma6L, derived from the healthy patient. For getting iPSC lines, in the fibroblasts of patients with the syndrome of prolonged QT- interval and an elongated spinal muscular atrophy episomal vector expressing genes OCT4, SOX2, KLF4, c-MYC via nukleofektsii was delivered. These genes are responsible for maintaining the pluripotent state. For differentiation to the cardio cells GiWi protocol was used, the duration of which takes 12 days [1]. However, for the mature cardiomyocytes in a number of protocols cells were kept in the post-differentiation conditions up to six months.

After differentiation, (day 11-12) cell monolayer formed visually, and about 30-50% of the layer surface contracted. Using flow cytometry, we counted the number of cells, which are positive for sarcomeric alpha-actinin. For if31-5 line (on day 16) it was 15.3%, for iSMA6L line (on day 20) - 14.6%. But it's worth noting that the cells did not survive for several months. As a control, cells were analyzed using immunocytochemistry. Staining was done on sarcomeric alpha-actinin (actinin), cardiac troponin T (cTnT) and myosin heavy chain (MHC). Figure 1 showed cells, differentiated from isma6L , with alpha-actinin (actinin) staining.

Also, on day 15 optical mapping of the differentiated cell monolayers was conducted. An excitation wave propagated over the entire surface of the monolayer, which allowed measuring critical stimulation frequencies for the tissue culture. The monolayers were removed and seeded as single cells to check for Patch Clamp. However, on a day 16 from starting differentiation procedure cells showed only potassium currents.

As the number of cells, which are positive for sarcomeric alpha-actinin for both cell lines were about 15%, it shows the stability of differentiation. In addition, it indicates the role of these cells in monolayer surface contractility function. However, from the other hand, the low presence of cardiac cells in the entire monolayer could correspond to notable inability of cells from both lines to survive for more than 50 days.

Interestingly, in contradistinction to other differentiation protocols, electro-mechanical syncytium formed already on the 15th day after differentiation. Considering patch-clamp results, it could show the main role of potassium channels to form the excitable tissue itself.

Murad Vagida
Researcher

Extracellular vesicles in patient with acute coronary syndrome

SCIENTIFIC ORGANIZATION

Moscow State University of Medicine and Dentistry named after A.I. Evdokimov

ABSTRACT

In our laboratory, we developed technique for detecting extracellular vesicles (EVs) by flow cytometry in blood of patients with acute coronary disease. We found that in blood the most abundant fraction of vesicles bearing CD41a-common platelet marker. CD41a+ fraction are 1.7-fold higher in patient group comparing to control (5,296 ± 2,590 vs. 3,069 ± 1,555; p=0.018). To monitor lymphocytes and extracellular components of atherosclerotic plaques we developed method for long-term cultivating plaque explants. In our in vitro model, the amount of T-cells become stable from 4 to 7 day.

KEYWORDS

Atherosclerosis, Extracelular vesicles, T-cells, Miocardial infarction, Acute Coronary syndrome.

ACKNOWLEDGEMENTS

This study was supported by the Grant of the of the Government of the Russian Federation, contract #14.B25.31.0016.

SUMMARY

INTRODUCTION

Atherosclerosis associated diseases is the one of the main cause of death in developed countries. Now it is well known that the formation of the atherosclerotic plaque is an inflammatory process in which are involved both cellular and extracellular components. T-cells are one of the main cellular conductor of this process [1]. The study of the pathology of atherosclerotic plaque are complicated by lack of adequate model of monitoring T-cells ex vivo in dynamic. We developed method to cultivating plaques in vitro.

Another crucial component are extracellular – cytokines and extracellular vesicles (EVs) [2] [3]. Many cell types release EVs into the blood stream, and these EVs may carry proteins characteristic of the cells that released them. Bulk analysis has shown that blood EVs carry tetraspanin CD63, which is expressed by cells of many types and is involved in the EV formation process [4]. Also, it has been reported that two molecules are common to blood EVs: CD41a, a platelet glycoprotein IIb/IIIa that is characteristic of platelets, and CD31, a cell adhesion molecule expressed by endothelia and less abundantly by other cell types.

By incorporating cellular proteins into their membranes, EVs may reflect not only the types of the cells from which they were released but also the physiological state of these cells [5]. Accordingly, EV composition may change in different pathologies, in particular in acute forms of coronary artery disease. The composition of EVs in the blood of patients with acute coronary syndromes (ACS) differs significantly from that found in healthy controls. For study EVs in blood of patient with ACS we developed flow cytometry – based method of phenotyping and enumeration of these particles.

MATERIAL AND METHODS

Blood collection

Peripheral blood was collected by intravenous withdrawal in vacuum tubes with sodium citrate as anticoagulant. Platelet poor plasma (PPP) was prepared within less than 1 h after blood collection by centrifugation at 3,000 g for 15 min. Then, plasma was aliquoted by 600 µl and frozen at -80ºC.

Coupling of monoclonal antibodies to magnetic nanoparticles

Monoclonal antibodies (Abs) against CD31, CD41a, and CD63 were dissolved in coupling buffer at a concentration of 2 mg/ml. For coupling, 1 mg of 15-nm iron oxide magnetic nanoparticles with carboxylic acid (MNPs) was incubated in 400 µl

of activation buffer. Afterwards, 400 µl of coupling buffer was added to activated MNPs followed by the addition of 1 mg of antibody and the mix was incubated for 2 h at room temperature. The reaction was stopped by addition of 10 µl of quenching solution and two washings on strong magnet. In order to visualize nanoparticles, prior to capture of the EVs we mixed the Abs–MNPs with fluorescent anti-mouse IgG1 Fab fragment. We washed away the unbound Fab fragments using a 100-kDa centrifugal device for two 5-min centrifugations at 1,100 g. Labeled Abs–MNPs were diluted in their initial volume with PBS.

Capture and detection of EVs with nanoparticles

PPP (100 µl, freshly thawed) was incubated with 60 µl of labeled Abs–MNPs for 1h at +4° C followed by addition of 2.5% antibody-based blocking reagent. The suspension of EVs conjugated to Abs–MNPs was labeled with fluorescent antibodies or isotype controls for 20 min at room temperature with continuous mixing. For CD31-coupled MNPs we used the following specific monoclonal antibodies: anti-CD41a-APC and anti-CD63-PE. For CD41a-coupled MNPs we used anti-CD31-AlexaFluor® 647 and anti-CD63-PE. For CD63-coupled MNPs we used anti-CD31-PE and anti-CD41a-APC. Afterwards, suspensions were transferred into magnetic columns mounted on an magnet separator. Unbound antibodies were washed away by gravity-mediated flowing of the input sample followed by the flowing of 500 µl of washing buffer for two times (PBS with 2 mM EDTA and 0.5% normal mouse serum). Then, magnetic columns were unmounted and EVs conjugated to Abs–MNPs were eluted with 2 x 400 µl of PBS and fixed with 200 µl of 4% formaldehyde solution. Directly prior to flow cytometry analysis, 50 µl of well-mixed counting beads were added. The procedure is summarized in Fig. 1.

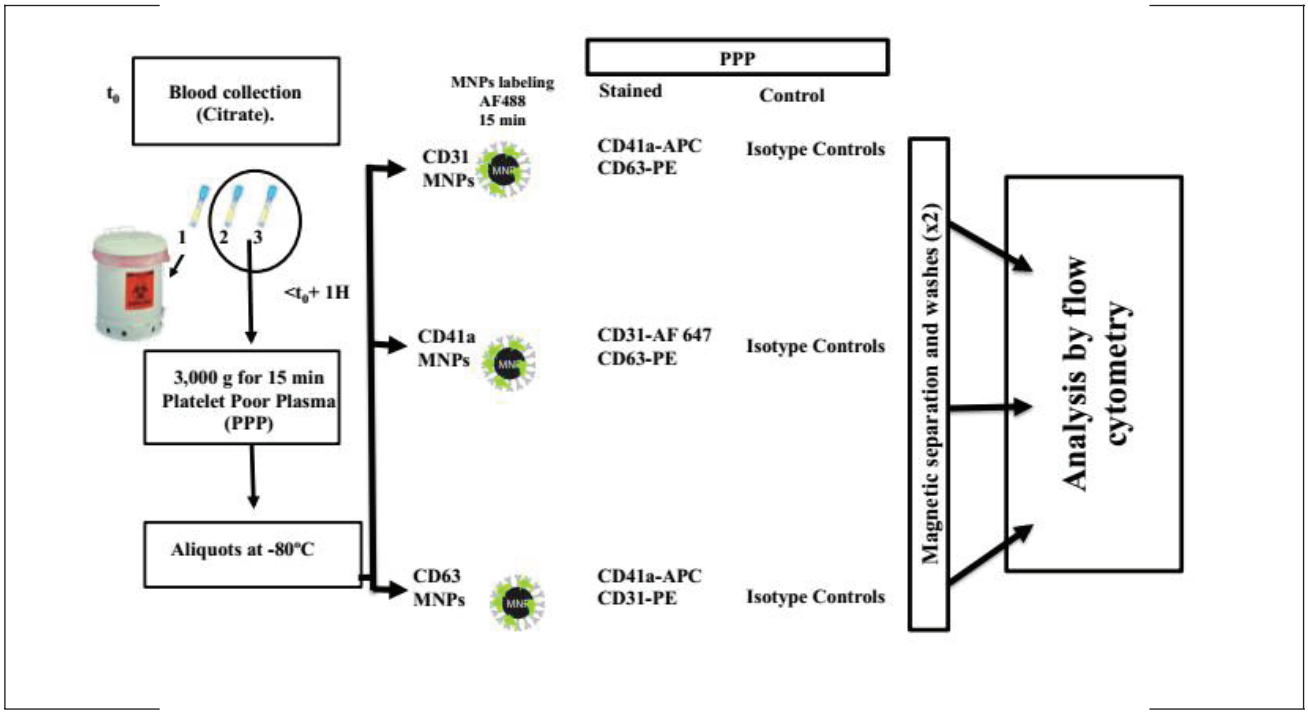


Fig 1. Summary of the protocol for capture and isolation of EVs

MNPs (15 nm) coupled to antibodies against one of EVs' antigens were incubated with EVs. MNPs were labeled by Fab_AF488 against the capture antibodies. Two other fluorescent antibodies were added to the captured EVs MNP–EV complexes were separated on magnetic columns and analyzed in a flow cytometer.

Flow cytometry analysis

Suspensions of EVs conjugated to Abs–MNPs were analyzed with a FACS Aria II SORP flow cytometer equipped with 355-, 407-, 488-, and 633-nm lasers. Fluorescence activated by the 488-nm laser set at a power of 180.3 mW and measured between 505 and 550 nm (Blue-525-channel) was set as the threshold. The flow cytometer sheath fluid was filtered through a series of in-line filters with nominal filtration rating of 100 nm and 40 nm. First, we acquired filtered PBS and set up the value of the threshold. We set fluorescence parameters in the highest voltage that maintained the positive peak of labeled Compensation Beads in the range of linearity of the trigger channel. We calculated compensation in FlowJo Software using single-stained CompBeads. EV events were counted in a single-event gate according to height and weight parameters of MNP fluorescence.

Cultivating plaque explants

Plaque explants were transported in sterile RPMI 1640 Advanced media with antibiotic/antimicotic. Parts of tissue without calcification or atheromatosis were cut perpendicularly on circular blocks with 2 mm thickness.

Blocks were cultured on collagen sponge in 35 mm petri dishes with 3 ml complete medium based on RPMI 1640 Advanced with added 1%-10mM non-essential amino-acids, 0.2%-100mM sodium pyruvate, Glutamine, antibiotic/antimicotic and 15% fetal bovine serum.

Collagen sponges were washed in complete medium prior using. Plaque were cultured in CO_2 incubator on 37°C, 5% CO_2. Each 3 days we replace medium.

Flow cytometry of cells from plaque

After weighing we cut tissues on blocks 2mm*2mm*2mm put them in enzyme solution (1,25 mg/ml collagenase from *Clostridium histolyticum* and 0,2 mg/ml DNAse I) and incubate on 37°C on shaker 1 hour 15 minutes. After, cell suspension was filtered through 40 mkm filter and washed in PBS.

Cells were labeled 15 minutes at room temperature with mixture of antibodies CD45-PE-Cy7, CD3-PerCP-Cy5.5, CD19-PE, CD4-APC-EFluor 780, CD8-eFluor 450. For exclusion of dead cells we used amino reactive dye Alexa Fluor 350.

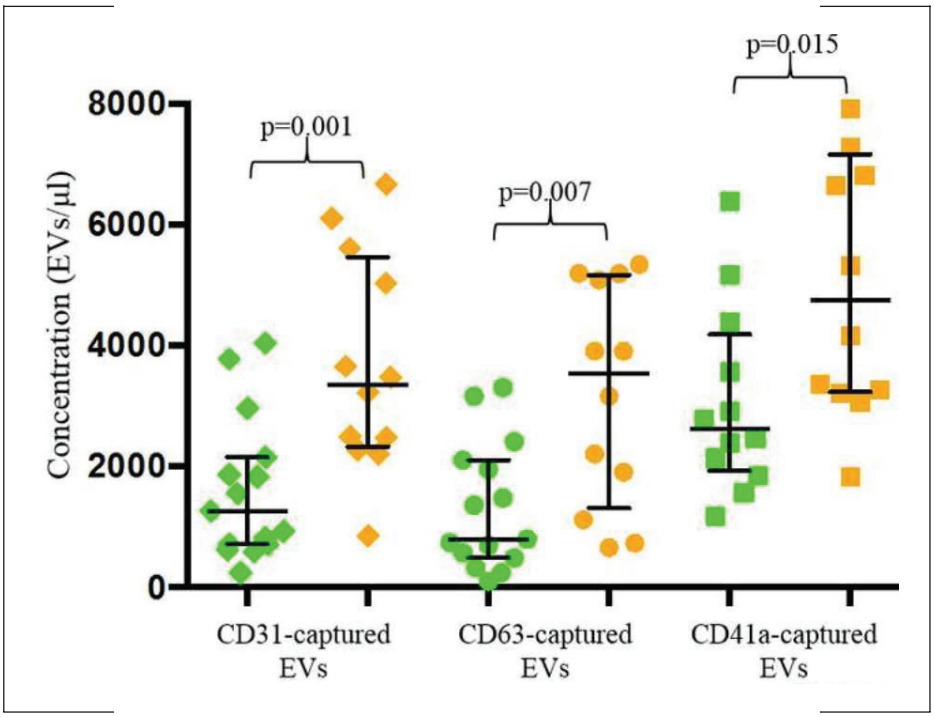
RESULTS

EVs in blood

We found that in blood of patients as well as in blood of healthy volunteers the most abundant fraction of vesicles was CD41a-positive. We showed that the total amounts of EVs captured by CD41a and positive for one or two of the detection antibodies were significantly higher than the amounts of CD31- and CD63-captured EVs (3,315 [2,411; 6,125] EVs/µl vs. 2,213 [859; 3,661] EVs/µl, p=0.035; vs. 1,908 [707; 3,308] EVs/µl, p=0.003, respectively).

With all the capture strategies used, the total amounts of EVs positive for one or two of the detection antibodies in ACS patients were significantly higher than in healthy volunteers. The amount of EVs captured by CD31–MNPs and positive for one or two of the detection antibodies in ACS patients was 3,359 [2,328; 5,472] EVs/l in comparison with 1,272 [714; 2,157] EVs/l in healthy volunteers (p=0.001). The total amount of EVs captured by CD63 in ACS patients in comparison with healthy volunteers was 3,541 [1,318; 5,173] EVs/µl vs. 806 [488; 2,112] EVs/µl (p=0.007). There were 4,752 [3,238; 7,173] EVs/µl in plasma of patients with ACS captured by CD41a–MNPs, whereas in plasma of healthy volunteers this number was significantly lower, 2,623 [1,927; 4,188] EVs/µl (p=0.015) (Fig. 2). For normally distributed data, we also compared the differences in means and found that in patients there was approximately a 2.4-fold higher amount of CD63-captured EVs (3,207 ± 1,827 vs. 1,321 ± 1,052; p=0.002) and a 1.7-fold higher amount of CD41a-captured EVs (5,296 ± 2,590 vs. 3,069 ± 1,555; p=0.018) than in healthy volunteers.

Fig. 2. Total amounts of EVs in blood of patients with ACS in comparison with healthy volunteers.



EVs from patients with ACS (brown symbols) and from healthy volunteers (green symbols) were captured with MNPs coupled to one of three Abs against CD31, CD41a, or CD63 and stained with the other two (fluorescent) Abs. Stained EV–MNP complexes were isolated on magnetic columns and subjected to flow analysis. EVs of different phenotypes have been enumerated. Data presented as dot plot with median and IQR.

We investigated whether the increase in EV concentrations in ACS patient plasma was restricted to a particular fraction of the EVs, or whether the numbers of EVs were proportionally increased in all antigenically different fractions of EVs that we tested. To answer this question, we enumerated EVs in three different subsets for all the captured populations: EVs captured by CD31-MNPs stained for CD41a and CD63, EVs captured by CD63-MNPs stained for CD31 and CD41a, and EVs captured by CD41a-MNP stained for CD31 and CD63.

The amounts of CD31-captured EVs of $CD41a^{+}CD63^{+}$ or $CD41a^{+}CD63^{-}$ phenotypes were significantly higher in ACS patients than in healthy volunteers (940 [456; 1,415] EVs/µl vs. 342 [246; 622] EVs/µl; p=0.009; and 2,133 [1,764; 4,211] EVs/µl vs. 761 [385; 1,807] EVs/µl; p=0.003, respectively). There were virtually no CD41a-negative vesicles among the CD31-captured EVs (Fig. 3).

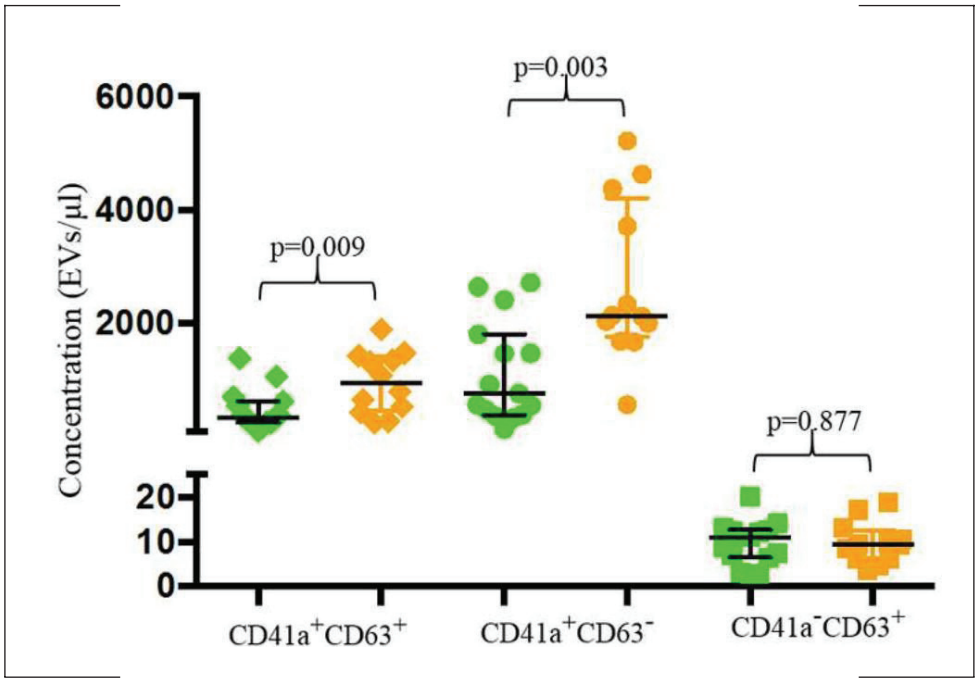
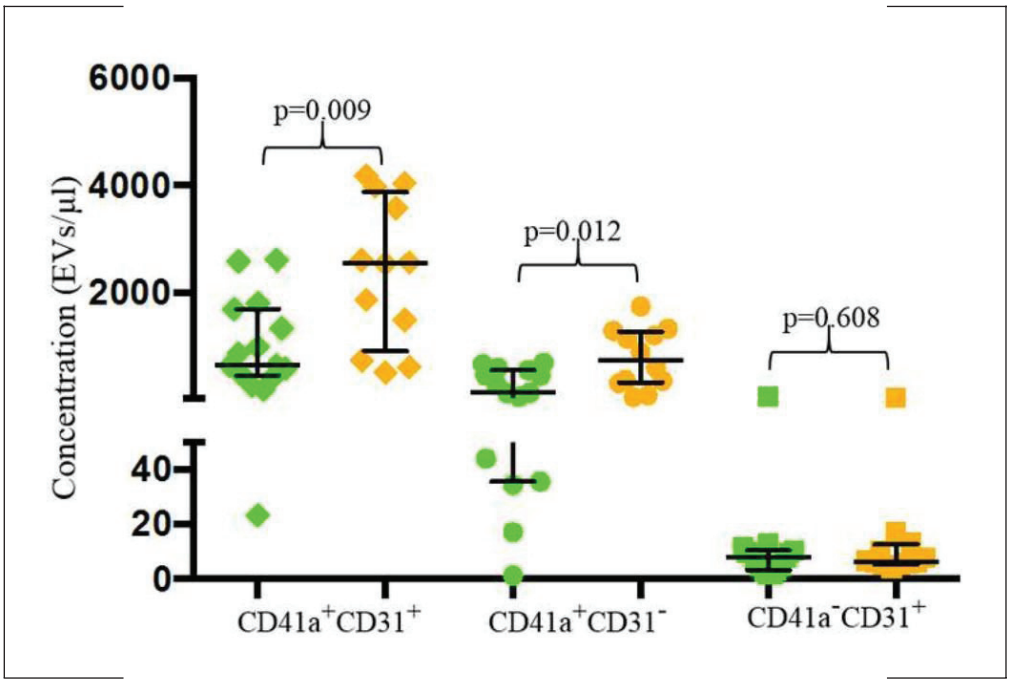


Fig. 3. CD31-captured EVs in blood of patients with ACS and healthy volunteers

EVs from patients with ACS (brown symbols) and from healthy volunteers (green symbols) were captured with MNPs coupled to Abs against CD31 and stained with fluorescent Abs against CD41a and CD63. Stained EV–MNP complexes were isolated on magnetic columns and subjected to flow analysis. EVs of different phenotypes have been enumerated. Data presented as dot plot with median and IQR.

There were almost no EVs of $CD31^{+}CD41a^{-}$ phenotype within EVs captured by CD63–MNPs and $CD41a^{+}$ fractions in ACS patients were significantly larger than in healthy volunteers (2,559 [931; 3,885] EVs/µl vs. 659 [463; 1,708] EVs/µl for $CD31^{+}$; p=0.009; and 758 [337; 1,282] EVs/µl vs. 147 [36; 568] EVs/µl for $CD31^{-}$; p=0.012, respectively) (Fig. 4).

Fig. 4. CD63-captured EVs in blood of patients with ACS and healthy volunteers



EVs from patients with ACS (brown symbols) and from healthy volunteers (green symbols) were captured with MNPs coupled to Abs against CD63 and stained with fluorescent Abs against CD41a and CD31. Stained EV–MNP complexes were isolated on magnetic columns and subjected to flow analysis. EVs of different phenotypes have been enumerated. Data presented as dot plot with median and IQR.

In all the fractions of EVs captured by CD41a–MNPs ($CD31^{+}CD63^{-}$, $CD31^{+}CD63^{+}$, and $CD31^{-}CD63^{+}$), we observed increased numbers of EVs in PPP of ACS patients compared with controls. However, only in the $CD31^{+}CD63^{-}$ fraction did this increase (almost two-fold) reach statistical significance (4,356 ± 2,391 EVs/µl vs. 2,199 ± 1,112 EVs/µl; *p*=0.010) (Fig.5).

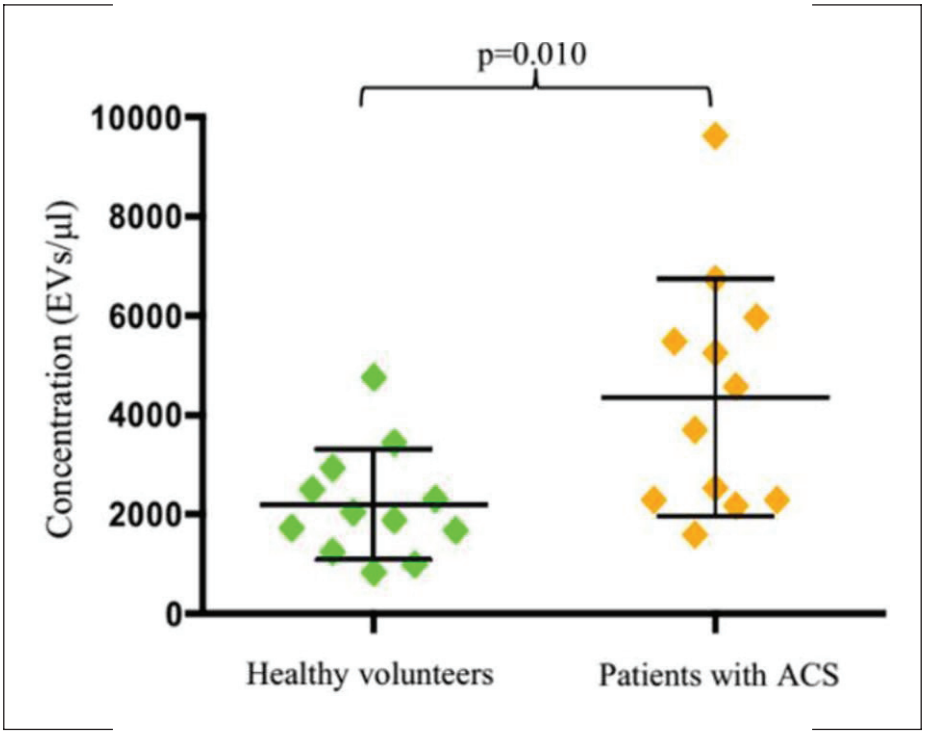


Fig. 5. CD41a-captured CD31+CD63- EVs in blood of patients with ACS and healthy volunteers

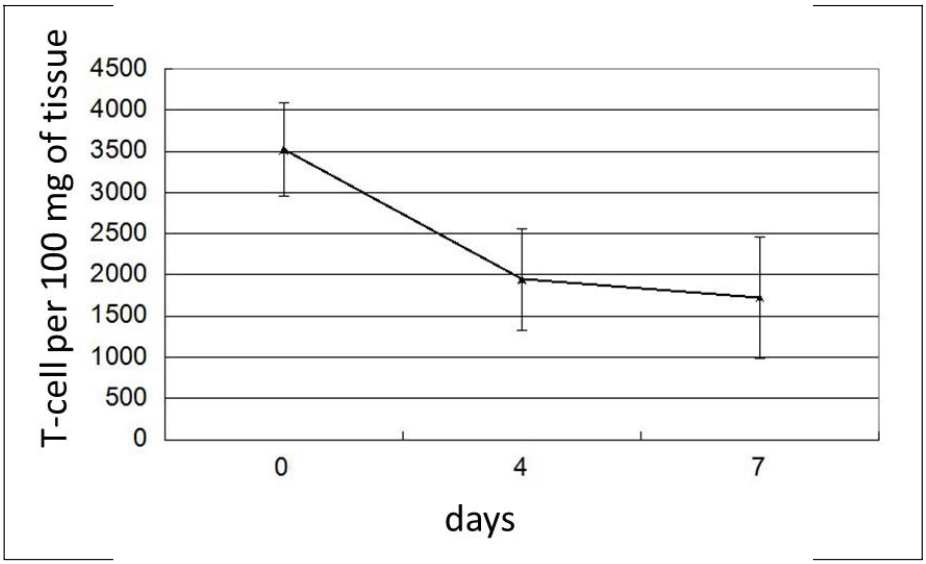


Fig.6. Dynamic of T-cells in cultured plaques. Data represented as M±m

EVs from patients with ACS (brown symbols) and from healthy volunteers (green symbols) were captured with MNPs coupled to Abs against CD41a and incubated with fluorescent Abs against CD31 and CD63. Stained EV–MNP complexes were isolated on magnetic columns and subjected to flow analysis. EVs of different phenotypes have been enumerated. Data presented as dot plot with mean ± SD.

Plaque explant in vitro cultivating

We found in ruptured plaque 54.65±7.34% CD4+ and 36.99±7.44% CD8+ T-cells compare to non-rupture 45.05±12.74% CD4+ and44.17±12.30% CD8+ T-cells. Ruptured plaques contain significantly high ($p<0.05$) number CD4+CD8- than non-rupture.

We analyzed T-cells in plaque in dynamic on days 0, 4 and 7. From 0 day to 4 there are tendency to decrease number of cells. After the fourth day the amount of cells are stabilized and live cells even could be detected on day 19 (Fig 6.).

CONCLUSION

In summary, we found that the predominant population of EVs captured through various antigens carry CD41a, indicating their platelet origin. The amounts of EVs were higher in the ACS patients than in controls. The increase in the numbers of EVs in the ACS patients does not occur across the board in all the EVs with different antigenic compositions, but rather is restricted to CD41a-positive vesicles, probably reflecting activated status of platelets associated with the disease.

We establish method for culturing atherosclerotic plaques in vitro

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Inhibitory GABA action in the neonatal mouse cortex in vivo

SCIENTIFIC ORGANIZATION

Kazan Federal University

KEYWORDS

Optogenetics, GABA, developing brain, inhibition, in vivo.

ACKNOWLEDGEMENTS

This work was supported by INSERM (LIA to RK), the grant to leading scientists (11.G34.31.0075 to RK), the program of competitive growth of Kazan Federal University, the subsidy allocated to Kazan Federal University for the state assignment in the sphere of scientific activities and RFBR (grant 14-04-01457 to MM).

SUMMARY

We present a novel optogenetic approach for the investigation of excitatory and inhibitory GABA actions in cortical neuronal networks using a mouse knock-in line with conditional expression of channelrhodopsin-2 (ChR2) in GABAergic interneurons. During whole-cell recordings from hippocampal and neocortical slices from postnatal day P2-15 mice, photostimulation caused depolarization and excitation of interneurons and evoked barrages of postsynaptic GABAergic currents. Excitatory/inhibitory GABA actions on pyramidal cells were assessed by monitoring the alteration in the frequency of excitatory postsynaptic currents (EPSCs) during photostimulation of interneurons. We found that in slices from P2-8 mice, photostimulation evoked an increase in EPSC frequency whereas in P9-15 mice, the response switched to a reduction in EPSC frequency indicating a developmental excitatory-to-inhibitory switch in GABA actions on glutamatergic neurons. Using a similar approach in urethane-anaesthetized animals *in vivo*, we found that photostimulation of interneurons reduces EPSC frequency at ages P3-9. Thus, expression of ChR2 in GABAergic interneurons of mice enables selective photostimulation of interneurons during the early postnatal period, and these mice display a developmental excitatory-to-inhibitory switch in GABA action in cortical slices *in vitro,* but so far show mainly inhibitory GABA actions on spontaneous EPSCs in the immature hippocampus and neocortex *in vivo*.

Valiullina Fliza
Junior Researcher

GABABR-dependent long-term depression at hippocampal synapses between CB1-positive interneurons and CA1 pyramidal cells

SCIENTIFIC ORGANIZATION

Kazan Federal University

ABSTRACT

Long-term plasticity at hippocampal excitatory synapses has been extensively examined. However, much less is known about long lasting changes in GABAergic inhibitory transmission. Although long-term plasticity at inhibitory synapses may have a major impact on hippocampal function. The goal of this study was to explore the nature of long term plasticity at the synapses between interneurons expressing CB1Rs (putative CCK+) and pyramidal neurons in the CA1 region of the hippocampus in vitro.

KEYWORDS

Inhibition, perisomatic, GABABR, plasticity, interneurons.

ACKNOWLEDGEMENTS

This work was supported by the program of competitive growth of Kazan Federal University and the Bundesministerium fr Bildung und Forschung (Bernstein Center for Computational Neurosciences 01GQ1003A).

SUMMARY

We used hippocampal slices (300 μm) which were prepared from the brains of 14–21 day-old WT (C57Bl6) mice. CA1 pyramidal cells were identified visually using IR-video microscopy. In paired recordings, presynaptic CB1+ putative basket cells were identified by location and firing pattern. The identity of the presynaptic neuron was further confirmed after finding the connected postsynaptic cell, by asynchronous release evoked by high frequency stimulation (10 action potentials 50 Hz) and the presence of depolarization induced suppression of inhibition. To extracellularly evoke synaptic currents, glass electrodes filled with ACSF were placed in the stratum pyramidale within -50–100 μm of the body of the recorded neuron. The theta burst stimulation protocol consisted of four bursts of five stimuli at 50 Hz separated by 200 ms. For LTD induction TBS was repeated 25 times.

For statistical analysis, the paired Student's t-test was used, and data are presented as mean ± SD.

According to the results of our data we found that TBS triggers robust LTD at CB1+ interneuron to pyramidal cell connections. The LTD induction is postsynaptic and requires activation of GABAB receptors. Also, we show that LTD at this connection involves GABABR-dependent suppression of adenylyl cyclase and consequent reduction of PKA activity. This contrasts markedly with other hippocampal synapses, where TBS typically induces LTP. Thus, functionally TBS-like activity will selectively suppresses CB1+ synapses and simultaneously promote other GABAergic inputs, which can have a strong modulatory impact on hippocampal network activity patterns.

Vasilenko Ekaterina

PhD-student

Researcher

Anti-TNF bispecific antibodies: functional properties

SCIENTIFIC ORGANIZATION

Lobachevsky State University of Nizhny Novgorod

ABSTRACT

Selective TNF blockade by bispecific reagents may become a promising strategy for the treatment of autoimmune diseases. Here we compared functional properties of anti-hTNF bispecific antibodies in vitro, as well as in vivo using a mouse model of lethal hepatotoxicity. Only BV-1 that could bind macrophage surface molecule F4/80 was able to block TNF produced from macrophages in vitro. The protective dose of BV-1 for 100% survival of humanized mice was at least half of the dose for BV-1c in vivo.

KEYWORDS

TNF, bispecific antibodies, macrophages, humanized mice.

Acknowledgements

This work was supported by the Russian Ministry of Science and Education (grant 14.Z50.31.0008) and Russian Science Foundation (grant 14-50-00060).

SUMMARY

Systemic TNF blockade is associated with the risk of undesirable side effects due to TNF role in host defense and in immune homeostasis [1, 2]. Previously it was reported that cellular sources of TNF specify its distinct functions in protective and autoreactive immune responses [3, 4]. It was shown that TNF derived from myeloid cells plays a non-redundant deleterious role in several disease models such as rheumatoid arthritis [5], severe sepsis, concanavalin A induced hepatitis [3] and EAE [4], making TNF from this cellular source a promising target for therapy.

For this purpose three anti-hTNF bispecific reagents were produced on the basis of unique single-domain antibodies (VHH) from camelids [6]. To ensure myeloid cell specificity, BV-1 combined anti-F4/80- and anti-hTNF-binding domains allowing a selective capture of hTNF secreted by monocytes/macrophages. Due to insertion

of several mutations into CDR- regions in F4/80-domain BV-1mut was unable to bind murine macrophages and therefore represented a reagent with systemic TNF-neutralizing activity. The third reagent was bispecific antibody BV-1c binding human TNF and lactoferrin. All bispecific proteins were expressed in *Rosetta 2 (DE3) pLysS E. coli* strain and purified by Ni-NTA liquid affinity chromatography.

The ability of these bispecific reagents to block TNF was tested by cytotoxic assay with WEHI 164 13 Cl cell line, sensitive to human TNF. According to the results, the following values of LD50 were obtained: 10 nM for BV-1, 15,5 nM for BV-1c and 57 nM for BV-1mut.

We also used cytotoxic assay to confirm the ability of BV-1 to specifically block TNF derived from myeloid cells. For this purpose we incubated macrophages derived from hTNFKI "humanized" mice with studied proteins and then incubated with LPS after washing step. After this we transferred the supernatant to WEHI cells. Survival curves showed dose-dependent neutralizing activity of BV-1 which provide complete WEHI cell survival in contrast to BV-1c and BV-1mut.

As myeloid cells are the principal source of deleterious TNF in mouse model of lethal LPS/D-Galactosamine (DGal) hepatotoxicity[3] this model was used to evaluate the activity ability to block TNF *in vivo*. 30 min prior to injection of hepatotoxic agents the following substances were administered to mice: phosphate-buffered saline (PBS) as negative control for survival (all animals in this group died) or murine monoclonal antibody F10 as positive control (all mice survived) or different doses of the experimental neutralizing agents. Kaplan-Meier survival curves were plotted and different concentrations of the bispecific antibodies were compared. For BV-1 the dosage provided 100% survival of the experimental animals was 1,5 μg/g while for BV-1c it was 3 μg/g.

These results demonstrate that selective inhibition of macrophage-derived TNF is more effective than systemic TNF blockade in the mouse model of lethal LPS/DGal hepatotoxicity.

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ADDITIONAL INFORMATION

Co-authors: Mokhonov V.V., Gorshkova E. N., Astrakhantseva I.V., Novikov D.V., Kruglov A. A., Tillib S.V., Efimov G. A., Nedospasov S.A.

Vitkin Alex

Professor - Department of Medical Biophysics & Radiation Oncology - University of Toronto

Development of new optical coherence tomography technologies to enable individualized cancer therapy

SCIENTIFIC ORGANIZATION

University of Toronto

ABSTRACT

Our biophotonics laboratory at the University of Toronto has recently joined forces with scientists and clinicians in Nizhnyi Novgorod to develop and use advanced biophotonic technologies for high-resolution structural and functional imaging of biological tissues, in an effort to enable personalized cancer medicine. The core technology is called optical coherence tomography (OCT), and our joint research efforts in this domain (technological, pre-clinical, and clinical) will be briefly described in this presentation.

KEYWORDS

Optical coherence tomography, cancer therapy.

ACKNOWLEDGEMENTS

The study was supported by the Russian Science Foundation grant No 14-15-00538.

SUMMARY

Despite considerable progress in, and impressive effectiveness of various non-invasive cancer treatments such as radiotherapy (RT) and chemotherapy (ChT), the clinical outcomes are somewhat variable because of the variation in individual patient responses. If some convenient measurements from specific patients undergoing specific treatments could be made that report on treatment progress and response, these could be used to select responders from non-responders, alter 'the doses' for the remaining treatment, and in general optimize the therapies based on individual treatment feedback.

In this Nighnyi Novgorod + Toronto collaboration, we are developing the enabling optical coherence tomography (OCT) imaging technologies and conducting preclinical and selected clinical studies to come up with quantifiable metrics of tumour and normal tissue responses to a variety of minimally invasive therapies. Specifically, the OCT imaging platform is being expended / refined to enable multiple modes of operation, including direct structural, polarization-sensitive, angiographic, and elastographic regimes. These yields unique high-resolution imaging information on tissue cellular organization, connective tissue compartment, blood microcirculation, and tissue hardness / stiffness, respectively. The ability of these multiple important and complimentary information channels to detect treatment-induced changes is investigated preclinically in a series of normal and tumour-bearing small animals (mice, hamsters) undergoing ChT, RT, and also photodynamic therapy (PDT). A series of treatment-specific multi-modal OCT response metrics are derived, and then tested in a series of further clinical pilot studies of PDT, RT and ChT in the pathologies of oral cavity and skin. Representative project results will be highlighted in this presentation. It is hoped that the multimodal OCT technologies and treatment response metrics thus developed will help usher in the era of "personalized cancer medicine" of the 21st century.

Vlasova Olga

Ph.D

Professor of the Department of Medical Physics, Deputy Head of the Laboratory of Molecular Neurodegeneration

SCIENTIFIC ORGANIZATION

Peter the Great St.Petersburg Polytechnic University

Use of optogenetic technology in cell culture models, implantable device to works in slices and live animals

ABSTRACT

Optogenetic is a powerful method that allows to modulate cellular physiological properties. In our article we demonstrate changes of electrical properties of cellular membranes on HEK-293T and hippocampal neurons transfected with channelrhodopsins and halorhodopsins induced by blue and orange light stimulation. In recent years, a method of developmental research has proved its effectiveness in the nerve cell stimulation tasks. In our article we demonstrate an implanted device for the stimulation of neurons in slices and live animals.

KEYWORDS

Optogenetic, Light stimulation, Neurons, Implantable device.

ACKNOWLEDGEMENTS

This work was supported by the megagrant N11.G34.31.0056, then by the Russian Scientific Fund grant 14-25-00024.

SUMMARY

Brain is one of the most complicated and poorly understood parts of the human body. There is a large group of disorders related to abnormalities in brain activity called neurodegenerative diseases. At the moment etiology and pathological basis of these diseases are unknown. That's why the fundamental assays in neurobiological field become more and more important. New technology that allows scientists to solve these biomolecular problems is called optogenetics. Optogenetics is a modern approach to modulate physiological status of excitable cells, including neurons. This modulation is achieved by combining the techniques of genetic engineering and photonics.

Cells of human embrionic kidney (line HEK-293T) are easily transfected so they are often used as an object of study. In our preliminary experiments HEK-293T cells were transfected with Channelrhodopsin and Halorhodopsin constructs. The responses were recorded using the patch-clamp technique in voltage clamp mode using blue and orange light stimulation.

After successful approbation on HEK cells, optogenetic experiments were conducted in mouse primary hippocampal neuron cultures. Neurons were transfected with ChR_2-GFP plasmidand stimulated by blue (470 nm) light. Traces of neurons activity were recorded in voltage and current clamp modes.

Brain functions studying requires neuron interface that could record parameters and stimulate brain with high time-space accuracy. Most researchers who use optogenetic method in laboratory conditions on in-vivo animals now use optical fiber that is sent through the implantable cannula .

Parameters of the pulses sequence and their generation is controlled by computer graphical interface or manual switch of modes.

Programmed LED control drivers ensure the setting of DC values for one or several separate LEDs or a cluster that consists of several diodes united in one output fiber. Each channel is controlled autonomously (manually in modes of CW, external TTL or analog modulation types) or by software installed on computer.

In department of Medical Physics in our Molecular Neurodegeneration Laboratory we are working on the development and testing of implantable device for monitoring of brain neurons physiological parameters (action potential).

Together with "Nano and Microsystem Technology" research laboratory we are developing a combined optical-electrode device that allows you to carry out combined research with the use of intravital microelectrode stimulation and optogenetic activation of genetically differentiated neurons.

Optrode allows to record electrical activity during optogenetic experiments. This combination of several microelectrodes allows you to record the activity of several neurons in light affected areas. It minimizes the effects of light diffusion inside the tissue and the mismatch of positions of the light source and the detector that records neurons excitation / inhibition parameters. An implant consists of the coaxial conical optical wave guide (optrode) integrated inside the implantable electrode array (multi-electrode array-MEA) for recording the experimental data.

Alzheimer's disease (AD) and aging are resulting in impaired ability to store memories, but the mechanisms responsible for these defects are poorly understood. It is known that electrophysiological response of mutant mouse neuron cultures in case of electrical stimulation results in significant decrease in frequency of action potentials [7]. Our future plans include use of optogenetics in slices and live animals from AD models. For these purposes we want to use the prototype of our optrode. Our future plans also include using the device in long-term experiments on the spinal cord motor neurons stimulation using optogenetic techniques.

Vysotski Eugene
PhD
Head of laboratory

Advances in bioluminescence mechanism of calcium-regulated photoproteins

SCIENTIFIC ORGANIZATION

Institute of Biophysics, Siberian Branch of the Russian Academy of Sciences; Siberian Federal University

ABSTRACT

Photoproteins represent a unique class of protein biochemistry. The spatial structures of several hydromedusan photoproteins, their ligand-dependent conformation states, and some their mutants with altered bioluminescence properties have been determined. Based on spatial structures and mutagenesis studies, a proton-relay mechanism for triggering the bioluminescence by Ca2+ was suggested. Mechanism provides qualitative rationalizations of many aspects of photoprotein bioluminescence as well as the function of residues of the substrate-binding cavity in this process.

KEYWORDS

Bioluminescence, photoprotein, coelenterazine, luciferase, calcium.

ACKNOWLEDGEMENTS

This work was supported by RFBR grants 12-04-91153 and 12-04-00131, the Program of the Government of the Russian Federation "Measures to Attract Leading Scientists to Russian Educational Institutions" (grant 11.G34.31.0058), the Program of the Russian Academy of Sciences "Molecular and Cellular Biology", and the grant of the President of the Russian Federation 'Leading Science School' (3951.2012.4).

SUMMARY

Bioluminescence is a widely distributed phenomenon among marine dwellers. Many of them generate light by oxidation of coelenterazine, an imidazopyrazinone derivative. Based on biochemistry of bioluminescence reactions, these coelenterazine-dependent luminous systems are divided into two classes. One is the luciferase-luciferin reaction in which enzyme catalyzes an oxidative decarboxylation of coelenterazine by O_2 with generation of a product, coelenteramide, in its excited electronic state. Another type is Ca^{2+}-regulated photoproteins, a unique class of protein biochemistry. The best known and studied among those are aequorin, first isolated from the jellyfish *Aequorea victoria*, and obelin, from the hydroid *Obelia longissima*. All photoproteins consist of a single polypeptide chain to which the oxygen-activated substrate, peroxy substituted coelenterazine, is stabilized by tight, non-covalent binding. Thus, photoproteins can be regarded as luciferases with a long-lived reaction intermediate. The Ca^{2+} binding to the protein initiates a final step of the reaction, decarboxylation of 2-hydroperoxycoelenterazine, leading to the generation of a protein-bound coelenteramide in its excited electronic state. Ca^{2+}-regulated photoproteins belong to EF-hand Ca^{2+}-binding proteins, one of

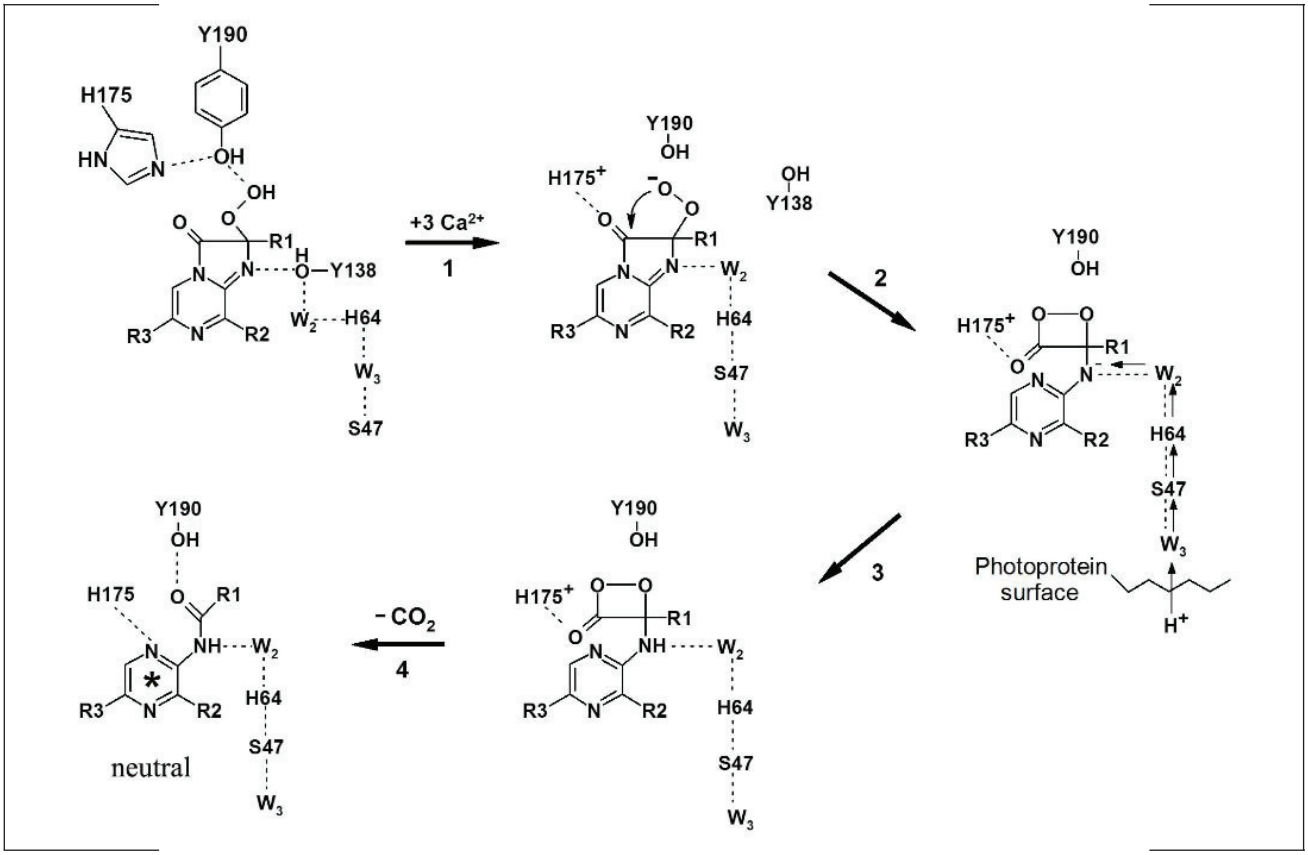
the most numerous and extensively studied protein families, because all of them contain three EF-hand Ca^{2+}-binding sites.

Over the past decade, the spatial structures of several hydromedusan photoproteins, their ligand-dependent conformation states, and some their mutants with altered bioluminescence properties have been determined. Based on these spatial structures and comprehensive mutagenesis studies, we proposed a proton-relay mechanism for triggering the bioluminescence reaction by Ca^{2+}. The suggested mechanism provides qualitative rationalizations of many aspects of photoprotein bioluminescence as well as the function of residues constituting the substrate-binding cavity in this process.

Bioluminescence is a widely distributed phenomenon among marine dwellers. Many of them generate light by oxidation of coelenterazine, an imidazopyrazinone derivative. Based on biochemistry of bioluminescence reactions, these coelenterazine-dependent luminous systems are divided into two classes. One is the luciferase-luciferin reaction in which enzyme catalyzes an oxidative decarboxylation of coelenterazine by O_2 with generation of a product, coelenteramide, in its excited electronic state. Another type is Ca^{2+}-regulated photoproteins, a unique class of protein biochemistry. The best known and studied among those are aequorin, first isolated from the jellyfish *Aequorea victoria*, and obelin, from the hydroid *Obelia longissima*. All photoproteins consist of a single polypeptide chain to which the oxygen-activated substrate, peroxy substituted coelenterazine, is stabilized by tight, non-covalent binding. Thus, photoproteins can be regarded as luciferases with a long-lived reaction intermediate. The Ca^{2+} binding to the protein initiates a final step of the reaction, decarboxylation of 2-hydroperoxycoelenterazine, leading to the generation of a protein-bound coelenteramide in its excited electronic state. Ca^{2+}-regulated photoproteins belong to EF-hand Ca^{2+}-binding proteins, one of the most numerous and extensively studied protein families, because all of them contain three EF-hand Ca^{2+}-binding sites.

Over the past decade, the spatial structures of several hydromedusan photoproteins, their ligand-dependent conformation states, and some their mutants with altered bioluminescence properties have been determined. Based on these spatial structures and comprehensive mutagenesis studies, we proposed a proton-relay mechanism for triggering the bioluminescence reaction by Ca^{2+} (Fig. 1).

Fig. 1. Proton-relay mechanism of the photoprotein Ca^{2+} trigger and formation of the primary product excited state.



The suggested mechanism provides qualitative rationalizations of many aspects of photoprotein bioluminescence as well as the function of residues constituting the substrate-binding cavity in this process.

Yudin Nikolay
Ph.D.
Senior Research Fellow

Race-specific distribution of the trpm8 gene variants: signs of selection

SCIENTIFIC ORGANIZATION

The Federal Research Center Institute of Cytology and Genetics the Siberian Branch of the Russian Academy of Sciences

ABSTRACT

A frequency distribution of the haplotypes at six SNPs in the TRPM8 gene sequences in Eurasia human populations has been studied. It is possible to assume that the prevalent fixation of the haplotypes with minor alleles of exon 7 in Asians is a Eurasian acquisition, which is more characteristic of the Eastern Asians as compared with the Western Asians. The separation of the European branch of the anatomically modern man out of Africa with a relatively low haplotype diversity at the TRPM8 gene was likely started in the Mesolithic and was fixed later.

KEYWORDS

TRPM8 gene, haplotype analysis, mRNA-isoforms, alternative translation, start codons.

ACKNOWLEDGEMENTS

This work has been done by the finance support of the Government of the Russian Federation (Project №14.B25.31.0033, Resolution No.220 Federation of April 9, 2010).

SUMMARY

A frequency distribution of the haplotypes at six SNPs in the *TRPM8* gene sequences in Eurasia human populations, including Russians, Altai Kazakhs and Tundra Chukchi has been studied. Four of six SNPs are in exon 7 and one disposes in exon 11. Both exons encode TRPM8 NH_2 domain fragments. The sixth SNP is localized in exon 23, encoding COOH domain fragment. The Chukchi and Russians display the most pronounced differences in pattern of diversity and frequencies of the some haplotypes. The main difference between the haplotype variants is determined by the SNP of exon 11, which gives the substitution Ser/Asn in the protein. The frequency of the overrepresentative Ser haplotype (H1) differ in the examined populations, amounting to 72% in Russians, 42.9% in Kazakhs and 24.6% in Chukchi. The Asn haplotypes carrying additionally the minor alleles at synonymous SNPs of exon 7 are characteristic for Asian populations: they spread with a total frequency about 31.2% in the Chukchi versus 10.2% in the Kazakhs and only 2,4% in the Russians. The frequency of all Asn haplotypes in the Africans is comparable to Chukchi; however, they have lesser 10% of the synonymous SNPs of exon 7. Molecular analysis of the six TRPM8 mRNA isoforms has shown that they are transcribed from the *TRPM8* gene H1 variant but have the different translation initiation sites which are generated by alternative splicing from TRPM8 pro-mRNA.

It is possible to assume that the prevalent fixation of the haplotypes with minor alleles of exon 7 in Asians is a Eurasian acquisition, which is more characteristic of the Eastern Asians as compared with the Western Asians. The separation of the European branch of the anatomically modern man out of Africa with a relatively low haplotype diversity at the *TRPM8* gene (mainly, with H1 haplotype) was likely started in the Mesolithic and was fixed later.

ADDITIONAL INFORMATION

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Doctor of science, Professor RAS

Director of Institute of Biomedical Technologies

New research directions in the Nizhny Novgorod State Medical Academy on the basis of the megagrant achivements

SCIENTIFIC ORGANIZATION

Nizhny Novgorod State Medical Academy

ABSTRACT

In 2010-2014 the project “Fluorescent proteins: novel approaches to the study of the mechanisms of physiological and pathological processes in living systems” was successfully completed. The project focused on the development and use of new approaches to the study of the molecular mechanisms of biological processes and targeted effects on living systems using the latest generation of fluorescent markers. Laboratory of fluorescence bioimaging successfully continuous work in the field of fluorescent proteins for cancer and stem cells research, and supported by new grants.

KEYWORDS

Fluorescent proteins, geneticallyencoded sensors for pH, H2O2, metabolic imaging, anticancer drug discovery.

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation (projekt 11.G34.31.0017), by the Russian Science Foundation (projects 14-15-00646, 14-25-00129).

SUMMARY

In 2010 the Nizhny Novgorod State Medical Academy (NNSMA) won the first megagrant competition, organized by the Government of the Russian Federation (Project № 11.G34.31.0017). As a result, a leading scientist Academician Sergey Anatolyevich Lukyanov organized **a new Laboratory of fluorescence bioimaging** in NNSMA.

In 2010-2014 the project “Fluorescent proteins: novel approaches to the study of the mechanisms of physiological and pathological processes in living systems” was successfully completed. The project focused on the development and use of new approaches to the study of the molecular mechanisms of biological processes and targeted effects on living systems using the latest generation of fluorescent markers**. Laboratory of fluorescence bioimaging** successfully works, has the world level, and covers almost all the main areas of biomedical researches in the field of fluorescent proteins - the development of technologies of monitoring living tumor cells using fluorescence microscopy and tomography; research opportunities of genetically encoded photosensitizers for targeted destroying cancer cells using cell lines and laboratory animals’ models; analysis of the dynamics of generation of reactive oxygen species in tumors using genetically encoded sensors of hydrogen peroxide, the development of methods of delivery of genetically encoded markers, sensors and photosensitizers to tumor cells in laboratory animals.

The laboratory is equipped with the unique equipment: the first in Russia system of molecular imaging IVIS Spectrum (Caliper Life Science, USA), a diffusion fluorescent scanner designed and developed in IAP RAS (Russia), the only in Russia a fluorescence microscope STORM (Nikon) with ultra-high resolution (of the order 20 nm). Address lab site: http://www.niipfm.nizhgma.ru/bioimidjing/.

The theme of megagrant was further developed and realized in two RSF projects:

RSF Project: 14-15-00646 Study of energy metabolism in cancer cells using genetically encoded pH-indicators and fluorescence bioimaging

The project aims to study the features of energy metabolism of tumor cells in vitro and in vivo models using fluorescence bioimaging techniques.

RSF project (researches performed by the laboratories) 14-25-00129. Development of advanced approaches to the studies of the mechanisms of action of anticancer drugs and early tumor response to the treatment based on optical and molecular technologies

The project aims to develop methods of analysis of early-response of tumor to drugs for pre-clinical studies.

2 PhD theses were defended on the theme of megagrant. 5 postgraduate students continue to develop the theme of megagrant.

In 2013 NNSMA won the third megagrant competition. A professor of the University of Toronto Alex Vitkin became a leading scientist and created another scientific **Laboratory of optical coherence tomography**. Established infrastructure for megagrant of Lukyanova SA (SPF vivarium, imaging systems) is effectively used for realization of megagrant of A. Vitkin. In 2013 **Institute of Biomedical Technologies** (http://www.niibmt.nizhgma.ru/) was established on the basis of two laboratories of megagrants. Nowadays Institute of Biomedical Technologies is a perspective, well-organized and working scientific institute, where students, postgraduate students and young researchers work on probation, work and gain professional skills. The Institute is funded by received grants and programs in the field of biophotonics, experimental oncology and regenerative medicine.

Zakharov Andrey
PhD
Research associate

Versatile interface framework development

SCIENTIFIC ORGANIZATION

Kazan (Volga region) Federal University

ABSTRACT

A universal platform for creating devices for the acquisition and processing of biopotentials (EEG, EMG, ECG) is developed. The system is designed to record brain (EEG) or muscle activity (EMG, EKG) and converting the signals into control actions for external devices. Also based on this platform it is possible to create interactive multi-purpose monitors of the state of human health.

KEYWORDS

Versatile framework, BCI, EEG, EMG, ECG.

ACKNOWLEDGEMENTS

This work was funded by the subsidy altocated to Kazan Federal University for the state assignment in the sphere of scientific activities.

SUMMARY

A universal platform for creating devices for the acquisition and processing of biopotentials (EEG, EMG, ECG) is developed. The system is designed to record brain (EEG) or muscle activity (EMG, EKG) and converting the signals into control actions for external devices. Also based on this platform it is possible to create interactive multi-purpose monitors of the state of human health.

The device arranged according to a modular principle and consists of the control communication module and optional remote modules. The control module (CM) based on the STM32F4xxx ARM microcontroller. These microcontrollers allow to vary the computing power and the price of the device without changing the printed circuit board. The CM can operate completely autonomously, powered by its own lithium-ion battery. The CM communicates with the computer via the USB interface with optional galvanic isolation (power and data) module. The CM also acts as a charger (USB) device to the battery. In autonomous mode CM can communicate with the PC, laptop or smartphone via WiFi interface. Also data can be recorded on microSD card.

The interface to the external modules contains: two high-speed serial peripheral interfaces (SPI); digital voltage supply 3.3 V; analog bipolar power-supply ±2.5 V; additional universal input/output ports (UIO). In digital mode the UIO can be used as clock or trigger, in analog mode – like ADC or DAC. It is possible to connect to the CM up to 4 ADC modules with a maximum frequency of digitization.

The overall dimensions of the CM are 6.5 x 5 x 1.5 cm (without shell and battery compartment). The device is supposed under Windows, Linux, Android operating systems; software for MacOS is developed.

At the moment, the converters based on the ADS1298 and ADS1299 are used as remote modules, with the following characteristics:

- ADC resolution 24 bit (provides speed and accuracy of measurements)

- 8 differential or 16 unipolar channels

- sampling rate 16 kHz (ADS1299, 1 kHz per channel) and 32 kHz (ADS1298, 2 kHz per channel),

- the amplitude of input noise 1 μv (ADS1299), 4 μv (ADS1298),

- programmable gain: 1, 2, 4, 6, 8, 12, (and 24 for ADS1299).

Biopotentials digitization options and the available data transfer capabilities provided by the described device allow to use it both in fundamental research and for clinical needs. The possibility of long-term data collection, including recording to the internal storage, give the potentiality of creation on the basis of the platform detailed diagnostics systems for cardiovascular, neurological diseases or abnormalities of the locomotor apparatus. Also highly configurable remote modules give capabilities for the comprehensive analysis of brain electrical activity (EEG) in the laboratory conditions that is required, for example, during brain-computer interfaces developing.

ADDITIONAL INFORMATION

Co-author: Alexandr Evstifeev.

Zhdanov Renad

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SCIENTIFIC ORGANIZATION

Institute of Fundamental Medicine and Biology

ABSTRACT

Title: Resilience to orthostasis and haemorrhage: A study of common genetic and conditioning mechanisms The objective of this study was to examine acquired and innate vagal mechanisms that protect against physical challenges and haemorrhages. These include examining change in heart rate variability in response to orthostatic challenge, platelet count (PLT), mean platelet volume, and single-nucleotide polymorphisms in genes. Regular physical training of athletes indirectly modifies the genetic predisposing effects of some haemostatic factors on vagal tone and reactivity.

KEYWORDS

Genetic predisposition, heart rate variability, haemostasis system at athlets and non-athlets.

SUMMARY

Abstract in full:

A major challenge presently is not only to identify the genetic polymorphisms increasing risk to diseases, but to also find out factors and mechanisms, which can counteract a risk genotype by developing a resilient phenotype. The objective of this study was to examine acquired and innate vagal mechanisms that protect against physical challenges and haemorrhages in 19 athletes and 61 non-athletes. These include examining change in heart rate variability (HF-HRV; an indicator of vagus activity) in response to orthostatic challenge, platelet count (PLT), mean platelet volume (MPV), and single-nucleotide polymorphisms in genes that encode several coagulation factors, PAI-1, and MTHFR. Individual differences in PLT and MPV were significant predictors, with opposite effects, of the profiles of the HF-HRV changes in response to orthostasis. Regular physical training of athletes indirectly (through MPV) modifies the genetic predisposing effects of

some haemostatic factors (PAI-1 and MTHFR) on vagal tone and reactivity. Individual differences in vagal tone were also associated with relationships between Factor 12 C46T and Factor 11 C22771T genes polymorphisms. This study showed that genetic predispositions for coagulation are modifiable. Its potential significance is promoting advanced protection against haemorrhages in a variety of traumas and injuries, especially in individuals with coagulation deficits.

Professor Dr. Renad Zhdanov's List of selected publications 2016-2014:

h-index = 14 - the data are extracted from the Web of Science® and reproduced under a license from Thomson Reuters): http://expertcorps.ru/science/whoiswho/info/45496 (Google Academia: 1652 citations, h-index 18 https://scholar.google.com/citations?user=myAUGaMAAAAJ&hl=ru)

Zhdanov R.I., Doinikova A.N., Jdanova S.I., Chernokhvostov Yu.S., Gadzhieva E.I., Dvoenosov V.G. Correlation between haemostatic and vegetate nervous system parameters under examination stress // Neuroscience and Behavioral Physiology. Springer. 2016. Vol. 46, № 3 . IF 0,400 (in press) as a translation of the published paper: Жданов Р.И., А.Н. Дойникова, С.И. Жданова, Ю.В. Чернохвостов и Э.С.Гаджиева, В.Г. Двоеносов. Корреляция параметров системы гемостаза и вегетативной нервной системы при экзаменационном стрессе // Журнал Высшей Нервной Деятельности им. И.П. Павлова. IF 0,400 – 2016. – Т. 66, № 2. – С. 202-208.

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Tryptophanyl-tRNA synthase gene expression as genetic marker of the athletes' overtraining // Geny I Kletki = Genes and Cells. 2015. – Vol X, # 3 (in Russian).

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Zheltukhin Andrey
Young researcher

Investigation of Life Span Extension by Torin-2 in the nematode Caenorhabditis elegans

SCIENTIFIC ORGANIZATION

Engelhardt Institute of Molecular Biology of the Russian Academy of Sciences

ABSTRACT

In this study we investigated effects of chemical inhibitor of TOR kinase torin-2 in the C. elegans model. We found that torin-2 is an efficient TOR inhibitor that directly inhibits TOR kinase affecting prs6 phosphorylation and inducing the autophagy, thus significantly extends the average lifespan.

KEYWORDS

TOR, aging, rapamycin, torin2.

SUMMARY

Serine-threonine specific protein kinase TOR is implicated as a major determinant driving the aging process, while its inhibition has a life-extension effect in different organisms, including flies, nematodes and mice. In the nematode model of Caenorhabditis elegans an inhibition of *let-363/CeTor* gene results in a significant increase in lifespan. Rapamycin, a natural small molecule inhibitor of TOR, has also potent life-extension activity in different organisms. In the present study we tested effects of the second-generation chemical inhibitor of TOR kinase torin-2 in the *C. elegans* model. Normal lifespan of the nematodes that have constant number of postmitotic cells is around 20 days. Sixty individual worms at the L4 stage were maintained in the nutrient agar medium supplemented with increasing concentrations of torin-2, up to 0.2 nM/ml. Another TOR inhibitor rapamycin was used as a control, along with TOR inhibition by RNAi, by feeding with bacteria carrying fragments of the *let-363/CeTor* gene. We found that torin-2 at the effective dose if 25nM/ml extends the average lifespan by 19,77%, rapamycin at the effective dose of 100 microM - by 20.15%, food deprivation - by 24.82%, as compared to the untreated control. The maximum lifespan was increased by 22.22% by torin-2, rapamycin and RNAi, and by 25.02% by the food deprivation. To study mechanisms of the torin-2 effects we monitored the ontogenesis, phosphorylation of the TOR-kinase substrate protein rsp6 and the autophagy. For the latter we used a genetic construct expressing the LC3 analog fused with GFP (LGG::GFP) that helps visualizing and counting autophagosomes. Animals were treated with as described above for 16 hours. Western blots with fractionated lysates of the nematodes developed with antibodies specific for GFP has revealed that torin-2 at 25 nM/ml increased the autophagy by 10%, at 100 nM/ml - by 20%, food deprivation - by 430%, RNAi - by 170%. Surprisingly, rapamycin at 100 microM/ml did not increase the autophagy. Western blots have demonstrated the reduction of rps6 protein phosphorylation by 20% with 25 nM/ml torin02, by 30% with 100 nM/ml torin-2, by 40% by food deprivation and by 60% by the RNAi. No reduction of prs6 phosphorylation was detected by rapamycin at 100 microM/ml. Torin-2 was also capable of 1.5-fold retardation of ontogenesis at 1 microM/ml, and a complete shut-of at 10 microM/ml, while rapamycin had barely detectable effect at 5000 microM/ml, and distinct non-specific toxic effects at higher doses.

Conclusion: Torin-2 is an efficient TOR inhibitor in the nematode model that directly inhibits TOR kinase affecting prs6 phosphorylation and inducing the autophagy. We also conclude that the effects of rapamycin described for other animal models might be different in nematodes, although the exact differences require additional studies.

ADDITIONAL INFORMATION

Co-autors: Kornev A. B. Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Chernogolovka, Russia. Chumakov P.M. If a positive answer to the conference application, please provide a poster report. Engelhardt Institute of Molecular Biology of the Russian Academy of Science, Moscow, Russia.

Zhivotovsky Boris
Dr. Sci, Professor
Professor and Head of laboratory

Chemoresistance of lung adenocarcinomas is regulated by Tudor staphylococcal nuclease

SCIENTIFIC ORGANIZATION

Lomonosov Moscow State University and Karolinska Institute

ABSTRACT

Lung cancer is the leading cause of cancer-related deaths worldwide. Non-small cell lung cancer (NSCLC), the major lung cancer subtype, is characterized by high resistance to chemotherapy.

KEYWORDS

Chemosensitivity, lung adenocarcinoma, mechanisms.

ACKNOWLEDGEMENTS

This study was supported by grant from the Russian Science Foundation (14-25-00056).

Summary

Lung cancer is the leading cause of cancer-related deaths worldwide. Non-small cell lung cancer (NSCLC), the major lung cancer subtype, is characterized by high resistance to chemotherapy. Here we demonstrate that Tudor staphylococcal nuclease (SND1 or TSN) is overexpressed in NSCLC cell lines and tissues, and is important for maintaining NSCLC chemoresistance. Downregulation of TSN by RNAi in NSCLC cells led to strong potentiation of cell death in response to cisplatin. Silencing of TSN was accompanied by a significant decrease in S100A11 expression at both mRNA and protein level. Downregulation of S100A11 by RNAi resulted in enhanced sensitivity of NSCLC cells to cisplatin, oxaliplatin and 5-fluouracil. $AACOCF_3$, a phospholipase A_2 (PLA_2) inhibitor, strongly abrogated chemosensitization upon silencing of S100A11 suggesting that PLA_2 inhibition by S100A11 governs the chemoresistance of NSCLC. Moreover, silencing of S100A11 stimulated mitochondrial superoxide production, which was decreased by $AACOCF_3$, as well as *N*-acetyl-*L*-cysteine, which also mimicked the effect of PLA_2 inhibitor on NSCLC chemosensitization upon S100A11 silencing. Thus, we present the novel TSN-S100A11-PLA_2 axis regulating superoxide-dependent apoptosis, triggered by platinum-based chemotherapeutic agents in NSCLC that may be targeted by innovative cancer therapies.

ADDITIONAL INFORMATION

A. Zagryazhskaya, I. B. Zborovskaya, and E. M. Tchevkina.

Zhukova Marina
Specialist
PhD student

Early Language Development of Children with a History of Institutionalization: from Behavior to Psychophysiology

SCIENTIFIC ORGANIZATION

Saint-Petersburg State University

ABSTRACT

The study focuses on neurophysiological and behavioral aspects of language development in children who are left without parental care and reside in institutions. Institutional settings are characterized by moderate to low quality of caregiving, therefore children are exposed to psychosocial deprivation that effects developmental trajectories in the variety of domains.

KEYWORDS

Language development, psychosocial deprivation, institutionalization, psychophysiology of language.

ACKNOWLEDGEMENTS

This research was supported by the Government of the Russian Federation (grant No 14.Z50.31.0027; E.L.G., Principal Investigator).

SUMMARY

Children left without parental care who are reared in institutional care have recently been shown to demonstrate an array of deficits and delays with respect to cognitive (Rutter, 2000; van IJzendoorn & Juffer, 2005) as well as social-emotional development (Bakermans-Kranenburg et al., 2012; Zeanah, et al., 2005). However, only few studies directly examined early communicative and language development of institutionalized children (IC). The existing body of research suggests that language development of IC children significantly lags behind that of their age peers raised in biological families (Windsor et al., 2011; Windsor, Moraru, Nelson, Fox, & Zeanah, 2013; Loman, 2009). Neuroimaging studied showed that IC children display reduced cortical volume (Chugani et al., 2001), white matter abnormalities (McLaughlin, et al., 2014) and atypical patterns of brain activity (Marshall, Reeb, Fox, 2008). Importantly, the neurophysiological aspects of language functioning have never been directly studied in this population of children, and most of the published behavioral studies focused on children aged 30 months and above, thus providing little information about earlier developmental stages.

In a set of empirical studies conducted by the Laboratory of Translational Sciences of Early Childhood at Saint-Petersburg State University, we are aiming to address these gaps in the literature by collecting complimentary datasets of behavioral and psychophysiological measures of language development in young IC children. During the talk, we will present an overview of the linguistic and neurophysiological parts of the project and present preliminary results illuminating significant language delays in young IC children, manifesting in both behavior (measured through CDI and PLS-5) and atypical neural responses (i.e., N400) to linguistic stimuli. We hypothesize that these delays and deficits can be linked to the suboptimal quality of early care and properties of the linguistic environment (e.g., insufficient quantity or quality of linguistic input) that these children are exposed to in their early lives.

Zvyagin Andrei

Doctor of Physico-mathematical Sciences

Head of laboratory

Biofunctional photoluminescent nanocomplexes for visualisation of intracellular molecular trafficking, diagnostics and therapy

SCIENTIFIC ORGANIZATION

Lobachevsky State University of Nizhni Novgorod - National Research University, Macquarie University

ABSTRACT

New biofunctional nanomaterials with exceptional photophysical properties afford new opportunities.Reported here fluorescent nanodiamonds (FND), nanorubies and upconversion nanoparticles (UCNP) were applied to visualise and probe biomolecular processes in live cells.The detection limit was pushed to the single receptor visualisation and tracking, so the post-activation fate of e.g.opioid receptor can be investigated.

KEYWORDS

Theranostics, nanobiotechnology, photoluminescent nanoparticles, biophotonics.

ACKNOWLEDGEMENTS

This work was supported by grant No. 14.Z50.31.0022.

SUMMARY

At the same time, the nanoparticle surface can host biofunctional surface moieties, enabling attachment of targeting and/or therpeutic cargo molecules.

These nanoparticle biocomplexes, such as FND-EGFP, nanoruby-(opioid ligand) or UCNP-(designed ankyrin repeat antibodies) are pieced together to form biohybrid nanocomplexes capable to enter cells or pathology lesions to enable diagnosis and therapy.

Development of new approaches for the diagnosis and therapy of tumours (taken together, termed theranostics) - one of the most dynamic areas of Biomedicine, where new nanomaterials afford new opportunities. The nanomaterial merits include: programmability of their physical and chemical properties; abundance of reactive functional groups on the surface; large effective surface area; optimum size, which determines preferential accumulation of nanoparticles in tumour tissue1. This paper reports on multifunctional theranostics agents based on a new-generation biofunctional photoluminescent nanoparticles with unique optical properties – fluorescent nanodiamonds2, nanorubies3 and upconversion nanoparticles4.

UCNPs in the form of hexagonal crystallites NaYF4 doped with Yb3+ and Er3+ or Tm3+ were synthesised in the size range of 20 – 100 nm by a modified solvothermal

Figure 1. (Top panel) TEM images of upconversion nanoparticles (UCNP). (c) Core-shell UCNPs coated with silica and loaded coatings and loaded with photosenstiser Rose Bengal (RB); Inset, UCNP@SiO2(RB) pelleted (left) and dispersed (right) in water.

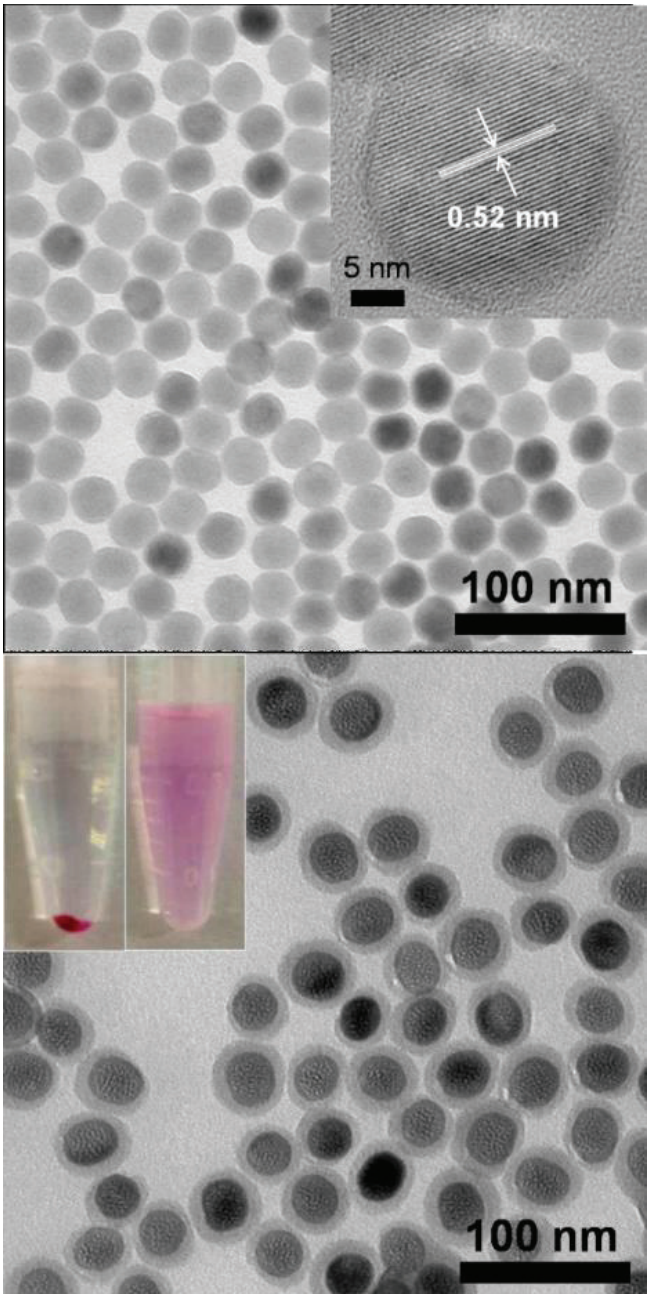
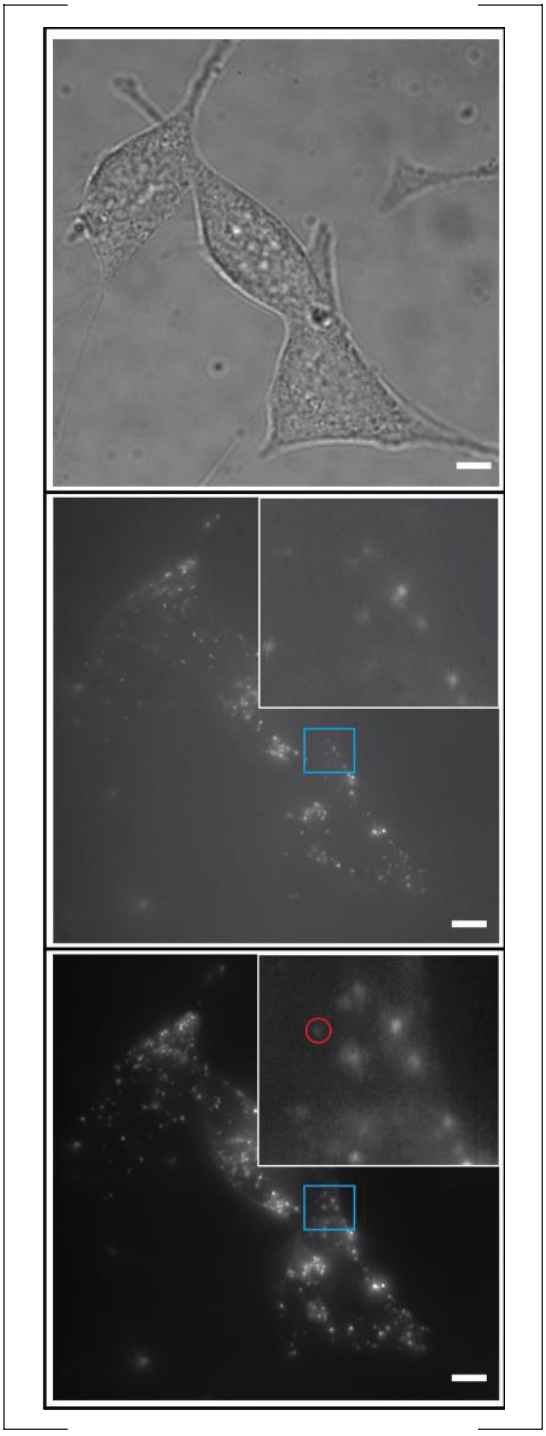


Figure 2. Microscopy images of AtT-20 cells incubated with nanorubies. (Top panel), (Middle panel) and (Bottom panel) show bright field, epi-luminescence and time-gated, background-free images. Insets show zoomed-in images as framed by blue squares. A red circle marks the nanoruby indiscernible in Middle panel. Scale bars, 10 μm.



method 5 [see Fig. 1(a,b)]. Nanorubies mean-sized 30 nm were produced by a femtosecond laser ablation method and high-energy ball milling, allowing the gram-scale, low-cost production3. Initially hydrophobic UCNPs were hydrophilised and coated with polymer or silica (Figure 1) 6. Surface-functionalised nanorubies appeared amenable to silane-based tethering of opioid receptor antibodies (Fig 2), such as designed ankyrin repeat proteins (DARPin)7 and mini-antibodies. We demonstrated binding of functional proteins by flexible design using solid surface peptide binding technology 6. The attachment of therapeutic vectors for photodynamic therapy, such as Rose Bengal6 and Killer Red, and immunotherapy, such as Exotoxin 7, were also developed and demonstrated.

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MACHINERY & ENERGY

Barakos George
PhD
Professor

Aerodynamic

SCIENTIFIC ORGANIZATION

University of Glasgow

ABSTRACT

This paper presents the development and application of transport-based transition models for CFD. Two challenging problems are addressed including flow at low Mach and high Reynolds numbers as well as problems at high transonic Mach and moderate Reynolds numbers. The work suggests that with proper calibration this family of models can provide results with good engineering accuracy.

KEYWORDS

CFD, Transition modelling.

ACKNOWLEDGEMENTS

Part of this work was supported by the EU F7 TFAST project.

SUMMARY

In this paper, the potential of transition prediction methods is explored for modelling transitional shock-wave/boundary-layer interactions. The study is fuelled by the strong interest of researchers and airframe manufacturers in reducing drag of vehicles flying at transonic speeds. The principle of drag reduction via flow laminarity is valid, provided there is no need for the flow to sustain large pressure gradients or shocks. This is true since laminar boundary layers are less resistant to flow separation. It is therefore worthwhile to assess the performance of CFD methods in modelling laminar boundary layers that can be tripped to turbulent just before the interaction with a shock. At this work, the CFD solver of Liverpool University is used. The method is strongly implicit and for this reason the implementation of 4-equation, intermittency-based models requires special attention. The Navier-Stokes equations, the transport equations of the kinetic energy of turbulence and the turbulent frequency are inverted at the same time as the transport equations for the flow intermittency and the momentum thickness Reynolds number. The result is stable and robust convergence even for complex 3D flow cases. The method is demonstrated for the flow around the V2C section of the TFAST EU, F7 project. The results suggest that the intermittency based model captures the fundamental physics of the interaction but verification and validation is needed to ensure that accurate results can be obtained.

Belyakov Nikolay
Master
PhD Student

The Effect of Water Droplets on Premixed Flames

SCIENTIFIC ORGANIZATION

Far Eastern Federal University

ABSTRACT

The aim of this work was the theoretical study of the effects of droplet sizes and concentration on burning velocity and extinction of premixed flames. The dependencies of the flame propagation velocity and the flammability limits on the properties of initial mixture with water droplets were obtained. The similarity of analyzed regimes of flame propagation with nonadiabatic flame propagation in narrow channel and with the flame stabilized in flat porous burner was discussed.

KEYWORDS

Fire safety, Extinction limit, Burning velocity.

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation (contract no. 14.Y26.31.0003).

SUMMARY

It is well known that water is an effective agent for fire extinguishing due to thermal effects related to the heat of vaporization. Specifically, the appropriately chosen water spraying can increase the flame suppression efficiency, which depends on the size of the droplets. For example, large particles can pass through the flame reaction zone with partial evaporation, and this effect leads to the increase of the water amount required for extinguishment. At the same time, small droplets can evaporate before the flame front and not create significant heat loss from the reaction zone required for flame extinction.

The aim of this work was the theoretical study of the effects of droplet sizes and concentration on burning velocity and extinction of premixed flames. The mathematical model used in this paper is an extension of the classical theory of laminar flame to the case of premixed flame with water particles. The model assumes that all droplets have the same size. It was assumed that droplets begin to evaporate when the temperature of the mixture attains the boiling point. Coefficient of heat losses spent on evaporation of the liquid depends on the size and concentration of droplets in the mixture. Depending on the value of heat losses and initial characteristics of liquid phase in fresh mixture, droplets can completely vaporize either before or behind the flame front. In this paper we take into account both cases as well as the transition between them.

In the case when droplets completely vaporize before flame front, using a partition into four areas: the first - fresh mixture heating zone from an initial to the boiling temperature; the second - the zone from the boiling temperature to the complete evaporation of the droplets; the third - the zone from the complete evaporation of the droplets to the flame front; the fourth - the zone of the combustion products.

In the case where the drops do not completely evaporate, flying via flame front, using the following partition into four areas: the first - fresh mixture heating zone from an initial to the boiling temperature; the second - the zone from the boiling temperature to the flame front; the third - the zone from the flame front to the complete evaporation of the droplets; the fourth - the zone of the combustion products without droplets.

The dependencies of the flame propagation velocity and the flammability limits on the properties of initial mixture with water droplets were obtained. The similarity of analyzed regimes of flame propagation with nonadiabatic flame propagation in narrow channel and with the flame stabilized in flat porous burner was discussed.

Demin Anatoly
Candidate of Sciences
leading scientific fellow

Solid Oxide Fuel Cells Based on Proton Electrolyte: Advantages, Problems and Achievements

SCIENTIFIC ORGANIZATION

Institute of high temperature Electrochemistry of the Ural branch of the Russian Academy of Sciences

ABSTRACT

A half-cell was fabricated using a tape calendering method with subsequent sintering. The single cell consisted of the 30 mm yttrium doped cerate-zirconate electrolyte (BCZY), the BCZY-Ni support, and the double cobaltite cathode. The cell exhibited very high OCV value: 1.141 V at 600 oC (ti=0.995) and 1.042 V at 700 oC (ti=0.98). These values were by 0.1 V higher than data reported in literature. The cell maximum power densities (174 and 280 mW cm2 at 600 and 700 oC, respectively) are acceptable for an intermediate-temperature operation and comparable with ones reported in literature.

KEYWORDS

Solid oxide conductors, protonic electrolytes, fuel cells, sensors, electrolyzers.

ACKNOWLEDGEMENTS

The results were achieved with support of the Ministry of Education and Science of the Russain Federation, contract # 14.Z50.31.0001.

SUMMARY

An interest to proton conductors is primarily aroused because in an SOFC based on proton electrolytes (SOFC-H) fed with hydrogen the fuel utilization (FU) is close to 100% whereas in the SOFC based on the oxygen-ion electrolyte (SOFC-O) FU is not more than 85 %. It was shown that the FU in the SOFC-H fed with methane is also high and exceeds 90% [1]. Thermodynamic analysis shows that an average electromotive force (EMF) in the SOFC-H is significantly higher than that in the SOFC-O [2]. Overall, the electrical efficiency of the former is by 15-20% higher than of the latter. It was shown that the efficiency of the methane fed SOFC-H is very high, especially at moderate relative power and can reach 80%.

However, proton electrolytes have some peculiarities that influence on the SOFC-H power and efficiency. Firstly, proton conductivity depends on p_{H2O}. Secondly, they have partial hole conductivity under oxidizing atmosphere. Our calculations show that increasing in hydrogen humidity leads to increase of the SOFC-H power whereas the air humidification does not affect the power. The calculations also show that even small hole conductivity leads to drastic decrease of the SOFC-H efficiency. So, if an average hole transfer number is 0.1, the SOFC-H efficiency is not higher than 50%.

In the frame of the Megagrant project, we fabricated half-sells using a tape calendering method (TCM) with subsequent sintering [3]. The single cell consisted of the 30 mm $BaCe_{0.5}Zr_{0.3}Y_{0.2}O_3$ (BCZY) electrolyte, the $Y_{0.8}Ca_{0.2}BaCo_4O_7$ cathode and the reduced 40%BCZY + 60%NiO and 45%BCZY + 55%NiO support and functional anode layers. It was found that the cell with BCZY electrolyte exhibited very high open circuit voltage (OCV) values (1.141 and 1.104 V at 600 and 700 ^oC) and therefore predominant ionic transport (average ions transport number 0.995 and 0.98 at 600 and 700 ^oC, correspondingly). These values are significantly higher than ones reported in literature for the cells with the similar electrolyte. For instance, the highest OCV values were obtained in [4] and they were by 0.1 V lower than ours. It is found that the maximal power densities of the fabricated cell (174 and 280 mW cm^2 at 600 and 700 ^oC, respectively) are acceptable for an intermediate-temperature range of operation and comparable with those reported in literature. The tape calendering method can be considered as effective strategy for SOFC-H fabrication, ensuring the formation of gas-tight electrolytes and acceptable electrochemical properties.

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ADDITIONAL INFORMATION

Co-author of the presentation: P. Tsiakaras, D. Medvedev, J. Lyagaeva.

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Simulation of thermoplastic composites

SCIENTIFIC ORGANIZATION

Skolkovo Institute of Science and Technology

ABSTRACT

This report considers the manufacturing of thermoplastic composites. The modeling of phase transitions in a material of thermoplastic matrix, taking into account changes in mechanical properties and additional shrinkage due to chemical reactions is performed. Equations for modeling of all key processes related to temperature cycle of thermoplast solidification are provided together with corresponding material constants, using polyetheretherketone (PEEK) as an example.

KEYWORDS

Thermoplastic composite, polyetheretherketone (PEEK), residual stresses, effect of crystallinity, failure criterion.

ACKNOWLEDGEMENTS

The part of this work was carried out in the Perm National Research Polytechnic University with support of the Government of Russian Federation (the Decree No. 220 on April 9, 2010) under the Contract No. 14.B25.310006, on June 24, 2013.

SUMMARY

Thermoplastic composites are gaining increasing popularity as a construction material in a modern industry. An essential feature of such materials is the ability to change its phase, turning into a viscous, near liquid state under high temperatures. All manufacturing processes of fabricating complex shaped components of thermoplastic materials involve heating and subsequent cooling of such materials. However, from a technology point of view, there is problem of warpage and deformations of structure occurring during phase transitions, accompanied by defects origination. Manufacturing experiments may be quite expensive and do not ensure required quality of final material. This necessitates the search for new methods allowing engineer to simulate manufacturing processes and the effects of temperature cycle on thermoplastic polymer. From a mathematical model point of view the main aspects are the changes in degree of crystallinity of material and related changes in mechanical characteristics, and additional chemical shrinkage. Therefore, material models to be developed shall account for following phenomena, depending on the phase state of material:

- growth of degree of crystallinity;
- changes in stiffness characteristics;
- changes in temperature properties;
- changes in strength properties of material.

Crystallization kinetics features a relatively well developed and, by all appearances, settled theoretical description [1–6]. Mechanical parameters of thermoplastic polymers can be found in various publications [1, 4, 5, 7]. The least developed area is a modeling of strength characteristics of such materials. Some attempts at evaluation of strength characteristics are described in [8–10]. In the present work a possible approach to modeling the influence of process temperatures on thermoplastic composites and evaluating residual stresses and strength characteristics is proposed.

Jimenez Garcia Antonio
PhD student
Student

Aerodynamic

SCIENTIFIC ORGANIZATION

University of Glasgow

ABSTRACT

This work is divided into two parts. The first is devoted to the analysis of the performance of a 1:5 model-scale ERICA tiltrotor in aeroplane mode configuration. For this case, numerical simulations are based on the Unsteady Reynolds Averaged Navier-Stokes equations, where the rotor blades were fully resolved. Uniform actuator disk is put forward to quantify the rotor effect on the total wing loads. The capability of the present CFD method in predicting the loads on the ERICA fuselage is investigated using a quasi-steady approach for the corridor and helicopter mode configurations.

KEYWORDS

CFD, Aerodynamic, Tiltrotor.

ACKNOWLEDGEMENTS

The use of the cluster Chadwick of the University of Liverpool is gratefully acknowledged. Some results were obtained using the EPSRC funded ARCHIE-WeSt High Performance Computer (www.archie-west.ac.uk) EPSRC grant no. EP/K000586/1. Part of this work is funded under the HiperTilt Project of the UK Technology Strategy Board and Leonardo Helicopters under Contract Nr. 101370. The authors would like to acknowledge the use of the NICETRIP experimental data and model geometry.

SUMMARY

Performance analysis of a 1:5 model-scale ERICA tiltrotor is presented, obtained using CFD. Three configurations, corresponding to minimum speed and high load for an aeroplane, corridor, and helicopter mode; are considered. For the aeroplane case, numerical simulations were based on the Unsteady Reynolds Averaged Navier-Stokes equations, where the rotor blades were fully resolved. The use of a uniform actuator disk was put forward as a means to quantify effect on the total loads. Comparisons with experimental data showed a good agreement and revealed the 4/rev. blade passage effect on the loads for the fully resolved approach. Results of the CFD with the uniform actuator disk also produced adequate estimates of the loads at the aerodynamic interaction zone.

The corridor and helicopter mode configurations were also computed using a uniform actuator disk. For the corridor case, results showed an excellent agreement with the experiment data at cross sections on the fuselage, fixed wing, and tiltable wing of the ERICA tiltrotor. The helicopter CFD predictions were in fair agreement with the DNW-LLF experiment on the fuselage and fixed wing, while the peak of CP distribution was under-predicted the region of aerodynamic interaction. The overall agreement with the experimental data demonstrated the capability of the present CFD method to accurately predict tiltrotor flows.

Kustov Oleg
Master

Peculiarity of experimental research of sound-absorbing liner specimens produced by 3D printing

SCIENTIFIC ORGANIZATION

Perm National Research Polytechnic University

ABSTRACT

Sound-absorbing liner specimens made of ABS plastic with honeycomb core and perforated plate were produced by 3D printing. These specimens were compared with those made of glass-fibre plastic and aluminum. Compared specimens have absolutely the same hole arrangements and perforated plate porosity (there was 24 variants in all). Experiments were carried out in impedance tube with normal incident waves. It was detected that sound-absorbing properties of specimens produced by 3D printing can be appreciably different from those made of standard materials.

KEYWORDS

3D printing; sound-absorbing liners; Helmholtz resonator; perforated plate porosity; impedance tube with normal incident waves; acoustic properties.

ACKNOWLEDGEMENTS

The work has been performed with the financial support of the Russian government under grant “Measures to Attract Leading Scientists to Russian Educational Institutions” (contract No. 14.Z50.31.0032).

SUMMARY

Fan noise propagating in ducts of bypass aircraft engine is suppressed with resonant acoustic liners. To design effective liner, in particular, a new resonator geometry, numerical simulation can be used [1, 2]. However, sound-absorption efficiency is verified by experiments carried out in grazing flow facility [3] or impedance tube with normal incident waves [4]. To determine acoustic properties of the liner on the first facility it is necessary to process experimental data by special numerical technique [5]. The transfer function method [4] used in impedance tube with normal incidence waves allows finding acoustic properties at once. The carrying out experiments encounters with a problem of specimen production, because technology for liners with a new-designed resonator geometry is not yet provided. Thus, 3D printing is a rational decision.

In this case, the production cycle includes designing specimen geometry in 3D modeling program, data translation into the format supported with 3D printer and finally 3D print of specimen. However, there are both strengths and weaknesses of 3D printing from ABS plastic. Its technology consists in layer-by-layer extrusion of ABS plastic fibers. There are two types of material used in 3D printer. The base material is ABSplus thermoplastic. The second material is to support base material by production of special layers at the necessary places. The support material is removed from the open areas by mechanical means, such as a screwdriver or stationery knife. From the hard-to-reach areas the support material is removed by dissolving with a special chemical composition.

Cell of the resonant liner is closed cavity with one or more holes with diameter of 1 mm. If cell is printed entirely with perforated plate and hard bottom plate, then all internal cavity is filled with support material. Because access to the interior of the cavity can be realized only through one hole, within a cell there is a stagnation zone, which complicates washing out the support material with liquid solvent. It causes too long time for dissolution of the support material, and in some cases it is absolutely impossible to remove completely support material. For the reasons outlined, it was decided to print specimens by parts with their following alignment in impedance tube. This approach allows variation of porosity of perforated plates and dimensions of the honeycomb cells.

Another limitation of this production method of liner specimens is minimum possible thickness of the wall. As each layer is formed of continuous filament, the 3D printer puts the filament in one direction, then turns around in the end of the segment and puts the filament in the opposite direction in order to move on to the

next part geometry. As a result, the minimum wall thickness of the honeycomb cells is not less than 1 mm.

To carry out experimental studies one-layer specimens were produced by 3D printing from ABS plastic. The inner volume of the specimen resonators is $5.2355 \cdot 10^{-6}$ and $1.5751 \cdot 10^{-6}$ m^3, and porosity of perforated plates is 5, 7 and 11 %. Comparison of 3D printed specimens was made with the honeycombs from standard materials. 3D printed and standard honeycomb cells were covered by either 3D perforated plate or plate from composite material. The thickness of the perforated plates and arrangement of the holes are the same.

As is known, the efficiency of the liner is described by acoustical impedance, which has to be correctly matched to the modal structure of the sound field, propagating in aircraft engine ducts. However, at the initial stage of the search of effective resonator geometry the estimation can be performed by sound absorption coefficient α. Its values were determined by measurements in an impedance tube with normal incident waves [6]. Experiments were carried out in the frequency range 500-6400 Hz at sound pressure level 140 dB.Obtained data have shown that sound absorption coefficient of the liner specimens produced by 3D printing from ABS plastic, can be differ by 0.2 from those for standard material liners, which is considerably. These results can be explained by different thickness of the specimen walls (it is 1 mm for 3D printing which exceeds wall thickness of honeycomb cell made of standard material) causing different wall stiffness and internal volume of the resonators.

Thus, one can conclude that production of promising liners by 3D printing can be used to experimental research of acoustic properties of the new resonator geometry, but consideration must be given to the fact, that properties of the produced liner specimens would be different from those produced by standard technology and with other materials. It is necessary to carefully select the 3D printer to produce liner specimens.

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ADDITIONAL INFORMATION

If you need the full version of abstract drawings and schedules, please contact us.

Latypov Ravil
Doctor of Science (Economics)
Professor

Research the termal efficiency and development of the ecological rotor motor applicable in agricultural farms

SCIENTIFIC ORGANIZATION

Kazan Cooperation Institute (RUC)

ABSTRACT

Present patented motor is external combustion engine operating on any fuel (firewood, sawdust, agricultural waste,manure, petro-waste, coal, etc). It produces mechanical and electric energy and hot air which could use for warning, drying,etc. in autonomous remote agricultural farms. The aim of this project is to manufucture such ecological motors.

KEYWORDS

Rotor motor, termal efficiency, heat exchange.

SUMMARY

There is well-known internal combustion rotor motor of professor Vankel. Present motor has oval-shape housing, equidistant rotor, which revolves on two shafts and divides internal space of motor into two chambers - “hot” and “cool”. Hot chamber is constantly heated by burner with any fuel. Some portion of the atmospheric air incomes in cool chamber and then compressed in heatexchanger. In determined position of the rotor hte input valve is opened and compressed air from the heatexchanger income to the inside red-hot surface of the housing, is expanded and rotor compresses next portion of atmospheric air to heate[changer. After working cycle output valve of the hot chamber is opened and hot air incomes to the heatexchangerand transfers heat to the next portion or air. Then some portion of air incomes to the burner for in full burning of the fuel and the rest of hot air could use for warnig, drying etc. Calculations show rising of the termal efficiency up to 40 % but it is necesary to experiment with the working models of the engine.

ADDITIONAL INFORMATION

Patent RF #2285124, #2319848.

Lomakin Evgeny
Doctor of Physical and Mathematical Sciences
Professor

Studies of properties of advanced structural materials and elaboration of mathematical models for the description of their behavior

SCIENTIFIC ORGANIZATION

Perm National Research Polytechnic University

ABSTRACT

The elaborations of mathematical models for the description of their mechanical behavior, fatigue and long-term properties, formulations of strength criteria are of scientific and practical meaning. One of scientific activities of laboratory of Mechanics of Advanced Structural and Functional Materials, Perm National Research Polytechnic University, is the elaborations of methods of experimental studies of mechanical properties of new structural and functional materials with the use of advanced testing machines and equipment.

KEYWORDS

Experimental mechanics, Elasticity, Plasticity, Fracture mechanics, Composites, Structural mechanics, Elastomeric materials, Mechanics of solids.

ACKNOWLEDGEMENTS

The work was carried out in the Perm National Research Polytechnic University with support of the Government of Russian Federation (The decree № 220 on April 9, 2010) under the Contract № 14.B25.310006, on June 24, 2013.

SUMMARY

The results of recent studies of deformation softening and post-critical deformation of steels are presented and the corresponding criteria are formulated for complex loading conditions. The elastic and strength properties of different grades of graphite materials as well as their fracture toughness properties are studied. The method for the determination of crack length and the values of fracture toughness characteristics of materials during stable equilibrium crack growth under bending conditions is considered. The unstable or non-equilibrium crack growth from short initial crack is observed in experiments, and corresponding theoretical explanation is given. The process of unstable crack growth is analyzed for different loading conditions. It has been shown that in the cases of short cracks, some part of stored energy transforms into kinetic energy, which can be described by the equation of energy balance during unstable crack growth.

Many structural materials, which are preferred for the developing of advanced constructions, are inhomogeneous ones. These materials have complex internal structure and properties, which make them to be more effectual in the solution of special problems required for development engineering. On the other hand, in consequence of this internal heterogeneity, they exhibit complex mechanical properties. In this work, the analysis of some features of the behavior of composite materials under different loading conditions is carried out. The dependence of nonlinear elastic response of composite materials on loading conditions is studied. Several approaches to model elastic nonlinearity such as different stiffness for particular type of loadings and nonlinear shear stress–strain relations are considered. Instead of a set of constant anisotropy coefficients, the anisotropy functions are introduced. Eventually, the combined constitutive relations are proposed to describe simultaneously two types of physical nonlinearities, one of which characterizes the nonlinearity of shear stress–strain dependency and another one determines the stress state susceptibility of material properties. The method for experimental determination of material's functions is proposed. Quite satisfactory correlation between the theoretical dependencies and the results of experimental studies is demonstrated.

ADDITIONAL INFORMATION

Valerii Wildemann.

Lombardi Pio

Dr.-Ing-

Research Manager

Multi Energy Systems within the smart grid era

SCIENTIFIC ORGANIZATION

Fraunhofer Institute IFF Magdeburg

ABSTRACT

The integration of volatile renewable energy sources, such as wind and sun, into the electric grid is the main challenge of the coming years. Multi Energy Systems (MES) may be a solution. In such systems the electricity generated by renewable energy sources is converted and stored in other forms such as gas and/or thermal. The stored electricity can be used for covering the electric and thermal loads as well as those due to the mobility. The speech aims to give an overview of the Multi Energy Systems pointing out the advantages of developing them within the era of smart grid.

KEYWORDS

Smart Grid, Renewable Energy Sources, Energy Storage Systems, Multi Energy Systems.

SUMMARY

The European energy strategy for the coming decades aims to increase to usage of Renewable Energy Sources (RES) for the generation of electric and thermal power. Among the RES, wind and solar energy will be the most used sources. By

2020 it is forecasted that 220 GW of wind power plants and 390 of photovoltaic plants will be installed in Europe However, these sources produce power not when it is demanded, but instead when particular meteorological conditions are met. Integrating the power generated by wind and solar into the electric network will be, therefore, a big challenge. It will involve the use of new solutions for optimally decoupling the power generated by renewable energy sources from the power demanded. Multi energy systems and virtual power plants are the most candidate solutions. Both of them contemplate the use of energy storage systems, as well as the use of demand side and demand response programs. In multi energy systems the stored power can be released in a different form compared to the original one. It is the case of the so called “power to gas” or “power to heat” storage solutions. In the “power to gas” the electric power is converted into gas (hydrogen and/or methane) and released into the natural gas infrastructure (pipelines, caverns). The “power to heat” the electric power is converted into hot water, steam or even ice and released into the thermal infrastructure (pipelines, storage).

The speech aims to point out the contribution which the multi energy system may give for integrating high amount of volatile renewable energy sources.

Maruta Kaoru
Doctor of Engineering
Professor

New concept combustion technologies with heat and mass recirculation

SCIENTIFIC ORGANIZATION

Tohoku University, Japan and Far Eastern Federal University

ABSTRACT

Research on effective energy conversion and combustion with new technology concepts are conducted in our research group. Effective heat and mass recirculations as well as combustion management and control allow increasing efficiency of combustion-based devices and reduce the pollutants. The main directions of our researches are as follows: • Micro-, Mild and Microgravity combustions • Flame structure diagnostic by micro flow reactor with prescribed temperature profile • Combustion with surrogate fuels, biomass, and synthetic fuels • Combustion in porous media.

KEYWORDS

Microcombustion, microgravity combustion, mild combustion, micro flow reactor, combustion in porous media.

ACKNOWLEDGEMENTS

The part of the study was supported financially by the Ministry of education and science of Russian Federation (project 14.Y26.31.0003).

SUMMARY

Three directions of researches on new concept combustion in extreme conditions will be introduced. These three directions are all based on common key concept, “combustion with heat and/or mass transfer managements.”

First, research and development on “microcombustion” are presented. Highly efficient Swiss roll microcombustor as general heating device and original new method “flame chromatography” for reaction kinetics study will be introduced. Second, fundamental combustion experiments conducted under microgravity environments for constructing comprehensive combustion limit theory will be presented. Discussion on the combustion limits which comprehensively cover both ordinary deflagration flame and peculiar phenomena termed “flame ball” is introduced. Finally, “high temperature oxygen combustion technology, HiTOx” which enables 40 % higher thermal efficiency compared with the ordinary heating furnace is introduced.

Minaev Sergey
Dr.
Head of Laboratory

Nonlinear flame front evolution equations

SCIENTIFIC ORGANIZATION

Far Eastern Federal University

ABSTRACT

Construction of the general fundamental theory of flame front evolution taking into account the strong nonlinear effects associated with the curvature of the front, the velocity gradients of the flow and the intrinsic diffusion-thermal instability essentially facilitates simulation of the combustion processes in flows with complex hydrodynamics.

KEYWORDS

Flame instability, thermo-diffusion, cellular flames, Lewis number.

ACKNOWLEDGEMENTS

The work was supported financially by the Ministry of education and science of Russian Federation (project 14.Y26.31.0003).

SUMMARY

In many cases, the flame is a complex dynamic system, which behavior may be explained by several mechanisms, either based on the kinetics of the reactions or other mechanisms, such as those associated with processes of selective diffusion or interaction with unsteady gas flows. For example, flame fluctuations may be caused by reaction kinetics or internal instability of the flame, the mechanism of which can be described by the simple reaction kinetics, but with inclusion of effects of the flame front curvature, the flow stretching, expansion of the combustion products, friction and heat transfer between the gas and the walls of the vessel and other factors. To highlight the mentioned mechanisms, the different types of flame instability is analysed at the basis of nonlinear evolution equations for the flame front that takes into account the strong nonlinear effects associated with the curvature of the front, the velocity gradients of the flow and the intrinsic diffusion-thermal instability. At the present time, the Markstein linear relationship between the local flame speed and the local flame front curvature is applied for modeling of the disturbed flame evolution. In case of flame, consisting of individual cells, or in the extreme case of a “flame ball”, this model is not able to describe such structures. During the project fulfillment, nonlinear evolution equations for the flame front and flame temperature were derived, which is able to describe both cellular and flat flame front propagation. The solution of this problem significantly improve the existing methods for effective simulations of flame evolution in complex flows with the same simplicity as “flamelet” model, but taking into account the nonlinear effects related with local curvature of the flame front and the nonuniformity of the gas flow. This problem is relevant in connection with the necessity of modeling the dynamic behavior of the flame front of practical fuel mixtures with large Lewis numbers, scintillation instability of SHS waves, oscillating fronts and traveling waves in the case of combustion of condensed materials.

Miroshnichenko Taisia
Master
Research fellow

Flame Behavior in Micro channels with Narrowing

SCIENTIFIC ORGANIZATION

Far Eastern Federal University

ABSTRACT

Flame propagation along the flow of gas flammable mixture into microchannel with smooth narrowing is studied in the present work. It is shown that flame can break through the narrowing zone even if its diameter is less than critical diameter for the given mixture. Features which influence on possibility of flame propagation depending on longitudinal size of narrow zone and flow velocity are studied.

KEYWORDS

Microchannel, critical diameter, flame quenching.

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation (contract no. 14.Y26.31.0003).

SUMMARY

Understanding of features of dynamical behavior of flame front in micro channels is necessary for developing of new gas burning technologies, such as burning of lean mixtures in porous media or micro combustion. It is necessary to create adequate models of flame propagation in channels with variable cross sections, nonhomogeneous temperature in walls and nonhomogeneous gas flow to develop small-size energy-transducing devices. It is well-known that flame can only propagate in channels with transverse diameter more than critical diameter. Critical diameter is usually considered as minimal diameter of indefinite channel where the flame propagation is possible. Critical diameter is usually considered as minimal diameter of indefinite channel where flame propagation is possible. Not only transverse size of a channel influences on flame propagation in micro devices, but its geometry and flow speed as well. The problem about flame propagation in the flow of inflammable mixture is solved in the present study. It is assumed that flame can freely propagate far from narrowing zone because diameter of the channel is more that critical diameter there. Diameter of narrowing zone is less than critical diameter. Data about gas flow velocity, length and diameter of narrowing, which influence on flame propagation limit, are gotten. It is shown that flame can pass through the narrowing even if transverse size is less than critical one, because time of heat exchange between chemical reaction zone and channel walls is limited and depends on the gas flow velocity. Critical diameter of narrowing depending on flow velocity and longitudinal size was constructed. Calculations are made in the frame of two-dimensional model with one-step chemical kinetics, which take into account structure of viscous flow and heat exchange between gas and channel walls.

Mokrin Sergey
Trainee researcher

Experimental Investigation of Flame Extinction Limit in Planar Microchannel

SCIENTIFIC ORGANIZATION

Far Eastern Federal University

ABSTRACT

The flammability limits of stretched flames stabilized in a planar microchannel were experimentally investigated. Lean methane-air premixture was used. Two opposite directed slot-jet burners and two quartz plates forming the planar microchannel allowed to reduce the influence of buoyancy effect and investigate the lean mixtures combustion at low values of stretched rate in conditions of normal gravity. Besides that, such system allows to investigate the effects related with heat recirculation from combustion products to unburned gas through the heat conducting channel walls.

KEYWORDS

Stretched flame, combustion in microchannel, flame extinction limit.

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation (contract no. 14.Y26.31.0003).

SUMMARY

The flammability limits of stretched flames stabilized in a planar microchannel with heat conducting walls were experimentally investigated in present work. Lean $0.6<\phi<0.8$ methane-air premixture was used. Original construction of the burning device consisting of two opposite directed slot-jet burners and two 50x50 mm and ~1.4 mm thickness quartz plates forming the planar microchannel allowed to reduce the influence of buoyancy effect and investigate the lean mixtures combustion at low values of stretched rate in conditions of normal gravity. Besides that, such system allows to investigate the effects related with heat recirculation from combustion products to unburned gas through the heat conducting channel walls.

The various regimes of combustion, such as flat flame, pulsating flame and also stable tubular flame at moderate values of stretched rate which was not observed previously were revealed during the investigation. The diagram of existence of various combustion regimes in dependence of stretched rate and equivalence ratio was plotted. The possibility of stable combustion of gas mixtures in such system at stretched rate values much smaller than limit value for ordinary stretched flames in conditions of normal gravity. Experimental results were verified by numerical simulations within the framework of one dimensional thermal-diffusive model taking into account the heat exchange between gas and channel walls and also the heat transfer through the channel walls.

Movchan Andrey
Professor, doctor of sciense
Head departament

Structure from shape memory alloys and stability problems

SCIENTIFIC ORGANIZATION

Institute of applied mechanics RAS

ABSTRACT

Shape memory alloys (SMA), due to their unique mechanical and thermal properties can be used to create unique designs and innovative technology. Briefly describes the known and planned uses of SMA in the medical, aerospace, energy, transportation, nuclear devices and fire safety. The necessity of adequate modeling of the thermomechanical behavior of the structural elements of the SMA.

KEYWORDS

Shape memory alloys, medical, aerospace, energy nuclear and fire safety, stability.

SUMMARY

Shape memory alloys (SMA), due to their unique mechanical and thermal properties can be used to create unique designs and innovative technology. Briefly describes the known and planned uses of SMA in the medical, aerospace, energy, transportation, nuclear devices and fire safety. The necessity of adequate modeling of the thermomechanical behavior of the structural elements of the SMA.

Particular attention is paid to the experimentally observed tendency of thin-walled elements of the SMA to the loss of stability caused by phase and structural transformations, if the latter come under the action of compressive stresses. It was found that the known elastic stability analysis methods can lead to an overestimation of multiple experimental values of maximum loads items from SMA. Critically evaluate different concepts, to adequately describe this phenomenon. This concept of “fixed load” and “variable load”, “ubiquitous additional phase

and structural transition," "universal additional phase transition in the absence of structural transformation" and "ubiquitous additional structural transformation in the absence of an additional phase transition." Analyzed uncoupled, coupled and coupled twice statements stability problem for the elements of the SMA. The problem of influence of small temperature perturbations in the analysis of the stability elements of the SMA is considered. It is shown that the smallest critical load values that work best with the experimental data obtained in the framework of the concept of "variable load" and once connected setting that corresponds to the assumption of isothermal nature of buckling. The assumption of adiabatic nature buckling leads to some increase in the limit loads, which, however, are significantly inferior in magnitude Euler buckling loads even in the case of martensitic, i.e. the lowest values of the elastic moduli. The solutions of the problems of stability of rods, plates and shells of SMA and interpretation of these solutions in the context of real projects of practical use of these materials are considered.

Obukhov Vladimir
PhD
Vice-director

Svotina Victoria
Head of Laboratory

SCIENTIFIC ORGANIZATION

Research Institute of Applied Mechanics and Electrodynamics (RIAME)

Radio-Frequency Ion Thruster Research and Development at MAI

ABSTRACT

The RIT Laboratory was founded at MAI in 2010. Under the supervision of Prof. H.W. a research team was formed, modern research and laboratory facilities were developed and constructed, and a family of RIT laboratory models was designed and tested during the period of 2010-2014. Based on the results of such tests, a number of contracts was concluded with industrial enterprises, including the Design Bureau "Fakel", TsNIIMash, and KBKhA. In 2014 the Laboratory became a completely self-financing one, and since then it has executed over 10 R&D works under the orders of the leading enterprises of the space industry of the Russian Federation and with their participation as the industry partners. During the whole period of the Laboratory existence, the total amount of its R&D works exceeded 100 million rubles. The Laboratory continues its woks successfully. According to available plans, in 2016-2020 the Laboratory will participate in the works within the frames of the Federal Space Program and other purpose-oriented programs.

KEYWORDS

Radio-Frequency Ion Thruster; Ion-Extraction System; Discharge Chamber; Mathematical Model; Power Processing Unit.

ACKNOWLEDGEMENTS

This work was supported by the Grant of the Russian Federation Government No. 11.G34.31.0022 for the state support of researches conducted under the supervision of the leading scientists at the Russian educational institutions of the higher professional education, which are gratefully acknowledged.

SUMMARY

The RIT Laboratory was founded at MAI in 2010. The research team of the Laboratory was formed during the period of 2010-2014 under the supervision of Prof. H.W. Loeb – the well known German scientist, who designed radio-frequency ion thrusters (RIT). Currently 6 candidates of sciences and 2 post-graduate students are among the members of this team. The foundation of the Laboratory made it possible to engage in work a team of young specialists, post-graduate students and students. Substantial financial support by the grant allowed creation of the modern research basis, laboratory facilities including. The production technology and testing principles were mastered as applied to the advance type of radio-frequency thrusters that did not have prototypes in the Russian Federation. Mathematical models for the operational processes in the thruster elements were developed, which allowed calculating electrophysical, thermal, and thermomechanical processes. Results of numerical modeling were used as a basis

for the design performance of RIT with the power of 0.3-45 kW. The laboratory models were designed and tested.

The interest to the results of activities of the \laboratory was exhibited by the industrial enterprises of space branch just since the first year of its existence. By the end of budgetary financing in 2013 the Laboratory executed 5 research works and 1 development project. Beginning from 2014, the Laboratory functions as a structural department of the Research Institute of Applied Mechanics and Electrodynamics of the Moscow Aviation Institute (RIAME MAI) under the self-financing conditions. During the period of 2014-2015 the Laboratory team members participated in the execution of 10 R&D works.

Along with the RIT development, the Laboratory solved the problems of RIT application and its integration with the spacecraft systems.

The following lines of activities were covered by the Laboratory:

- Performance study and design optimization for the RIT model with the power of up to 2kW provided with the ion-extraction system made of the carbon-composite materials.
- Development of high-power RIT and study of its characteristics, design optimization for its primary units and for the RF discharge power supply system.
- Research, development and test-bench optimization of the low-power radio-frequency ion thrusters.
- Analytical and experimental study for the physical and technical problems and elaboration of proposals on the development of onboard means for the contactless action on large-sized debris objects for their removal from operational orbits.
- Definition of design proposals on the complex development of maneuver schemes for multiple removals of space debris objects from the GEO region to the disposal orbit with the use of a service spacecraft and onboard means for contactless impact on uncooperative space objects.
- Ballistic analysis for the trajectories of emergency crew return from the lunar satellite orbit to the Earth, and development of software for calculating trajectories for transfer to the Moon and libration points of the Earth-Moon system.
- Investigation for a possibility of using a EP-powered spacecraft for a contactless impact on the low-orbit uncooperative space debris objects for changing their orbit altitude.
- Investigation and development of numerical methods for modeling the processes of radio wave propagation in the communication radio-channels of deep-space spacecraft with electric propulsions onboard, and analysis of noise immunity of onboard radio systems.
- Research aimed at the development of several options for a lunar takeoff and landing manned spacecraft and a lunar landing cargo vehicle as a security for lunar missions.
- Study for the problems of development of ground test complexes for modeling the effects of EP influence on the systems of spacecraft designed for the Solar system exploration.
- Calculation of nominal trajectories for the primary and reserve launch windows. Analysis of ballistic possibilities to parry nonstandard situations related to the temporal impossibility of standard use for an electric propulsion system (EPS).
- Development of engineering design procedures and software for the problems of inserting spacecraft with apogee EPS into the GEO.
- Development of mathematical models and software; mathematical modeling for the a spacecraft insertion into the GEO with the use of AEPS, test studies for the AEPS influence on different spacecraft parts, elaboration of recommendations on minimizing the AEPS effect on various parts of spacecraft being a part of the “Yenisey-A1” space complex.
- Development of methods and software to optimize trajectories of SC with EPS to the planets of earth group and asteroids.

- Designing of radio-frequency ion thrusters of new generation on the basis of analytical and test studies, and their testing.
- Elaboration of proposals on the design and engineering appearance aspects of the service spacecraft and input data for formulating technical requirements for a project on the development of space complex as related to an onboard cruise compensating EPS and onboard system for the injection of ion beam as a means for a contactless impact on the objects of space debris as applied to the space platforms designed by the Reshetnev Company “Information Satellite Systems”.
- Development of technical requirements to the design characteristics and elaboration of recommendations on solving the problems of EPS development for a non-expendable lunar tug on the basis of comparative analysis for various EP types.
- Comparative analysis for the efficiency of transport operations in space on the basis of application of power supply and propulsion complexes comprising solar and nuclear power plants.
- Comparative design analysis for various options of inhabited lunar basis and substantiation for the stages of its construction.
- The grant of the President of the Russian Federation in support of the activities of the leading scientific schools of the Russian Federation HSh-143.2012.8 “Fundamental studies for the physical processes in electric propulsion thrusters of next generation as applied to space missions in the near and deep space”.
- The grant of the President of the Russian Federation in support of the activities of the leading scientific schools of the Russian Federation HSh-895.2014.8 “Fundamental studies for the physical processes in electric propulsion thrusters of next generation as applied to space missions in the near and deep space”.

Research and development activities were executed under the contracts with the enterprises of the rocket-and-space industry: Keldysh Research Center, TSNIIMASH, Lavochkin Research and Production Association, Experimental Design Bureau “Fakel”, KBKhA, Reshetnev Company “Information Satellite Systems”.

During the whole period of the Laboratory existence, the total amount of its R&D works exceeded 100 million rubles. The Laboratory continues its woks successfully. According to available plans, in 2016-2020 the Laboratory will participate in the works within the frames of the Federal Space Program of the Russian Federation and other purpose-oriented programs.

ADDITIONAL INFORMATION

Co-author: Svotina Victoria, Head of Laboratory, RIAME MAI. If a positive answer to the conference application, please provide oral report.

Palchikovskiy Vadim
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New anechoic chamber for aeroacoustic research: development, qualification tests, use in experiments

SCIENTIFIC ORGANIZATION

Perm National Research Polytechnic University

ABSTRACT

The paper presents principal stages of development and use in aeroacoustic research a new anechoic chamber built in Perm National Research Polytechnic University in 2014-2015. It is shown some design features of the anechoic chamber and results of its qualification tests. The rigs built for generation of aerodynamic noise sources in the anechoic chamber are considered. Quality assessment of the anechoic chamber in measurements of turbulent jet noise, vortex ring noise and in localization of the noise sources of spinning sound field is carried out.

KEYWORDS

Anechoic chamber, acoustic wedges, reverberation room, impedance tube, qualification tests, air turbulent jet, vortex ring generator, aeroacoustic research.

ACKNOWLEDGEMENTS

The work has been performed with the financial support of the Russian government under grant “Measures to Attract Leading Scientists to Russian Educational Institutions” (contract No. 14.Z50.31.0032).

SUMMARY

The environmental noise of aircrafts is a key issue in their competitiveness. To satisfy future noise standards it is necessary to create brand-new solutions based on deep scientific research, development of efficient methods and techniques of noise source identification and suppressing. Experimental studies are powerful means for reaching mentioned tasks. Laboratory conditions allow performing experimental studies in the controlled environment, in addition, there is not required high financial, time and human resources as with full-scale tests. However, to ensure reliable experimental data in laboratory research it is necessary to provide the free-field acoustic conditions, i.e. sound propagation as if there are no reflections from the walls. Such a facility is called an anechoic chamber.

In 2014-2015, the anechoic chamber has been designed and built in Perm National Research Polytechnic University (PNRPU) for small-scale experimental studies on jet noise, vortex ring noise and other problems associated with aeronautical acoustics. It should be noted that at present the only other analogous operating facility in Russia is anechoic chamber AC-2 of Central Aerohydrodynamic Institute (TsAGI) built in 1970s, which also enables experiments with small-scale models.

The PNRPU anechoic chamber with concrete walls of 40 cm thickness is a well-isolated room from external noise and vibrations. The walls, ceiling and floor inside the chamber are lined with sound-absorbing wedges from basalt superfine fibers in acoustically transparent glass cloth [1]. The materials used for the acoustic treatment are inflammable, thus ensuring fire safety of the chamber. The chamber also ensures requirements on ventilation and lighting. To make the chamber easy-to-use the following additional rooms were designed and built: apparatus room; room for preparing equipment to experiments; room for fan units of the jet rig; special room for vortex ring generator, which installed into the wall of the anechoic chamber.

The sound-absorbing wedges have width 20 cm, length 100 cm, and total height 80 cm. The optimal density of basalt fibers has been chosen in a series of experiments with the wedges in reverberation chambers of TsAGI [2] and it is 30 kg/m^3. The wedges are assembled in blocks of five wedges inserted into a thin metal wireframe (diameter of the wire is 2 mm) to preserve the geometrical parameters of the structure.

To determine the frequency lower limit of the wedges the impedance tube has been built. It has a cross section of 0.4 m x 0.4 m and a length of 5.2 m. The transfer function method [3] used in the PNRPU impedance tube determined that the absorption coefficient of the wedges is equal to 0.99 and above starting with

130 Hz. However, final data on the sound-absorbing ability of the lining could be found in qualification tests of the anechoic chamber.

The qualification tests were carried out according to ISO 3745 [4]. They consisted in determination of the maximum allowable radius between a test source and a measurement location where inverse square law spreading holds, within some tolerance. This radius determines the region in the anechoic chamber where quantitative acoustic measurements can be performed without suffering from the reflection of sound from the walls of the chamber, i.e. in the free-field conditions.

To study the acoustic quality of the anechoic chamber in PNRPU, three sound sources were used:

- low-frequency 15”-loudspeaker (100 - 2000 Hz);

- omnidirectional source Bruel & Kjaer 4295 (low and medium frequencies 125 - 5000 Hz);

- high-frequency sound source based on the compressor driver JBL Selenium D408 Ti (5000 - 20000 Hz).

With these sound sources, two types of experiments were performed. In the first case, the source was placed near a wall, in the region of the expected noise source of a turbulent jet, which will be present in the chamber. In the second case, the source was placed in the center of the anechoic chamber, which corresponds to the typical tests of acoustic characteristics for pieces of machinery.

The measurements in both cases were performed for three radial directions 0^{O}, 45^{O} and 90^{O} from the source. For this purpose the traverse microphone system was built in the chamber. The acoustic data were obtained by moving microphones in discrete steps along a radial, with the microphones motionless during data acquisition (30 s) at each microphone location. Then the source was replaced and the measurements were repeated.

The performed measurements have shown that the anechoic chamber in PNRPU realizes the free-field conditions. The radius of the region where the inverse square law spreading is observed equals to 3 m in the frequency range 125 Hz – 20 kHz, provided that microphones are at least at the distance of 1 m from the wedge tips.

To carry out in the chamber research involving noise generation by aerodynamic sources the jet rig and vortex ring generator were designed and built. The jet rig reaches velocity equal to 200 m/s with nozzle exit diameter of 8 cm. Two fans connected in series supply air jet into the chamber and pullout the air through collector. Each fan has frequency converter and jet velocity can smoothly be controlled with PC software from apparatus room. Fans stand outside the chamber in isolated room. To prevent pass of fan self-noise into the anechoic chamber there are silencers in the air ducts. The measurements in the PNRPU anechoic chamber have shown that spectra of turbulent jet noise are the same trends as those of known jet rigs [5].

For research of vortex ring, which is a simplest aeroacoustic object, the vortex ring generator was built. The experiments carried out in the anechoic chamber have shown that vortex ring noise can be determined on initial path of vortex ring motion even at background noise of the generator [6]. In spectrum there is a narrow frequency range where acoustical pressure is maximum, that is typical of vortex ring. Subsequent motion of the vortex ring leads to shift this pressure maximum in lower frequencies. Observed effects are in good according to those obtained earlier in anechoic chamber AC-2 TsAGI [7]. Thus, obtained results show that PNRPU anechoic chamber can be used in fine aeroacoustic experiments.

The built chamber was also used in experiments on spinning acoustic mode identification [8]. This problem associated with development of effective liners for suppressing aircraft fan noise. Experimental determination of the modal structure can be made with a microphone array mounted inside or outside the duct. In performed research, a planar microphone array placed outside the inlet duct has been used for measuring spinning acoustic modes, and the obtained data were processed with the beamforming method. Spinning modes were produced by a special generator based on the inlet of PS-90 turbofan engine. Sound was generated by 34 acoustic drivers JBL 2451H placed around the circumference under the test facility. Tests were carried out without flow.

The measurement results show that spinning mode is located at a point, which position depends on the mode number (this phenomenon is similar to the results

obtained with planar beamforming method for propeller or open rotor noise [9]). There was also not detected any reflections distorting the noise locations. It indicates that the anechoic chamber can be used in experiments on localization of the noise sources.

In conclusion one can say that designing and building PNRPU anechoic chamber led to restore of domestic capacities in the development and production of wedges for large anechoic chambers. Performed tests demonstrate that the anechoic chamber allows the aeroacoustic measurements to be performed to obtain quantitative results.

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ADDITIONAL INFORMATION

V.F. Kopiev, V.V. Palchikovskiy, I.V. Belyaev, Yu.V. Bersenev, S.Yu. Makashov, M.Yu. Zaitsev, I.V. Khramtsov, O.Yu. Kustov, T.A. Viskova, I.A. Korin, E.V. Sorokin.

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Increasing the hydraulic and thermal efficiency of transport heat exchangers

SCIENTIFIC ORGANIZATION

Kazan National Research Technical University named after A.N.Tupolev

ABSTRACT

We present a review on heat transfer equipment of modern heavy vehicles. Heat exchanger characteristics can be improved through the use of heat transfer insifiers - vortex generators, swirling devices, microsctructurized surfaces. We show efficiency of heat transfer enhancement methods on the basis of numerical and experimental studies. We present recommendations on their use. We show their influence on the performance of the engines on the example of EGR cooler.

KEYWORDS

Heat transfer, hydraulic resistance, intensification, heat exchangers.

ACKNOWLEDGEMENTS

The work under the contract 14.Z50.31.0003 under the supervision of leading scientists S.A.Isaev.

SUMMARY

Block 1 - Numerical studies:

1.1. We proposed and substantiated the concept of composite grids constructed by intersecting multiscale structured mesh topology with a simple substitution of unstructured overlay inserts zones. We have developed a generator of 2-2.5 D composite meshes.

1.2. We spent improving the accuracy and computational efficiency is developing a package of hydrodynamic and thermal profile of VP2/3 and sigma-Flow through the introduction and adaptation Demidov library for algebraic accelerator convergence of the iterative process.

1.3. We performed verification modified 2003 Rodi-Leshtsiner-Isaev model shear stress transfer in compared with the forecasts on models of different levels and the experimental data, in particular obtained by the project at the Institute of Mechanics, Moscow State University.

Block 2 - Heat transfer enhancement - numerical and experimental studies:

2.1. We have proposed and numerically substantiated the new form of the surface vortex generator - elongated oval dimple, which is thermal and thermal-hydraulic efficiency significantly superior to traditional spherical and cylindrical wells at an intensification of turbulent heat transfer in a narrow channel. We studied the properties of an elongated oval dimple in the wall of the narrow channel. We found a tendency to increase the maximum in modulus of the transverse flow velocity in a channel with oval dimple elongating fixed spot area and the depth values of the order to the weight average speed in the channel. With the broadening of the oval dimple we found a tendency to laminar vortex flow in the channel. Size separation zone in the upper wells sharply reduced with a decrease in the width of the oval dimple and virtually the entire hole gets filled with swirling flow.

2.2. Based on the results of experimental research and analysis of the literature on the flow resistance and heat transfer medium pipes and channels with the systems of spherical projections:

- We have identified the mechanisms of intensification of heat transfer and the border of the laminar-turbulent transition;

- We found that the intensification of heat transfer in these pipes is up to 1.89 in the range of small numbers Re = 200-2200 with an increase in the hydraulic resistance to 1.97. In the transition range of Reynolds numbers Re = 800-2100 intensification of heat transfer in these pipes is up to 6.98 with an increase in the hydraulic resistance to 6.82 times. When Reynolds number Re = 5000-100000 intensification of heat transfer in these pipes is up to 2.89 with an increase in the hydraulic resistance to 6.7;

- We have identified the impact of the major operating and geometrical parameters in the coefficient of hydraulic resistance and heat transfer coefficient. We got generalizing dependences for calculation of hydraulic resistance and heat transfer for turbulent flow regime.

2.3. On the basis of the pilot study, we have formed a data bank on the coefficients of hydraulic resistance and heat transfer medium flat channels with one-sided arrangement of cylindrical dimples. On the basis of an integrated experimental and numerical studies, we have developed guidelines for the calculation of hydraulic resistance and heat-transfer channels with cylindrical dimples. We have established the effect of regime parameters of the flow and design parameters intensifiers on hydraulic resistance and heat transfer channels with cylindrical dimples. We got generalizing dependences for calculation of hydraulic resistance coefficients and heat transfer medium, describing the experimental data in the laminar and turbulent regimes with a tolerance of ± 10% at a confidence level of 0.95. We performed a numerical study of flow and heat transfer in channels with cylindrical dimples with package VP2/3. We showed a satisfactory agreement on the thermal-hydraulic efficiency of the results of numerical and experimental studies. We have shown that patterns of behavior of thermal and hydraulic performance as a whole do not differ from those of channel characteristics and bears the spherical dimples.

2.4. We continued the study of heat transfer and hydrodynamics in the flow of spherical dimples. On the basis of the restructuring jet-wave structure with increasing depth of the spherical dimples in the wall of a narrow plane-parallel channel with a fully developed turbulent flow of an incompressible fluid is proposed map mode it separated flow for a fixed Reynolds number 40000. Special attention was paid to the intensification of mono tornado-like swirling flow in the dimple, which is formed when transition from symmetric to asymmetric flow.

2.5. We have received the influence of dimensionless geometrical and operational parameters on the hydraulic resistance of bundles with different layout on the surface of the spherical dimples.

2.6. We have singled out the cork, wave, ring, dispersed and threadlike flow regimes with visual study of the structure of air-water flow in the tubes with inserted tape. Visualization of the flow of boiling freon confirmed the existence of threadlike streams on the tape and heat conditions. We have found that a discrete placing on the tape edges at an angle to the axis of the belt shifts the belt to the liquid surface of the heat exchange tube, which favorably affects the characteristics of the boiling process.

We experimentally investigated the heat transfer and hydraulic resistance of tubes with a variety of twisted tapes at boiling Freon. On the basis of experimental studies found that when calculating the coefficient of heat transfer in channels with embedded smooth and ribbed twisted tapes with forced convection R134a can be used Manglik-Bergles relation and Giniyatullins relation obtained for water. We studied the effect of regime parameters on heat transfer during boiling of refrigerant R134a in channels with twisted tape. We noted that a greater impact on the change of heat transfer provides the heat load delivered to the work site. We found no effect of the Reynolds number in the range of 31000 ÷ 83000. The increase in heat transfer coefficient occurs with a decrease in the relative step twist, due to the growing influence of mass forces. Intensification of heat transfer in channels with twisted tape relatively straight channel without inserts on average for y = 3 to 1.61; y = 4 to 1.51; 6 and y = 1.42. We got a generalization relationship to calculate the heat loss at boiling refrigerant R134a in channels with embedded smooth twisted tapes.

Block 3 - Studies of heat exchangers:

3.1. We conducted tests of laboratory samples of shell and tube heat exchangers with surface heat transfer intensifiers in the form of spherical and annular projections for various combinations of pairs of working fluids in a wide range of regime parameters for fixed overall weight and size characteristics:

- We got an increase in power of heat exchangers with intensifiers heat in the form of spherical or annular projections at a turbulent flow regime (Re = 4000-20000) in the tubes to 1.25-1.37 times during the growth of the hydraulic resistance in the heat exchange system of tubes up to 1.1 -1.6 times;

- We found an increase of heat power of heat exchangers with intensifiers in the form of spherical and annular projections in the transition Reynolds number (Re =

1000-4000) to 1,45-2,85 times during the growth of the hydraulic resistance in the heat exchange system of tubes up to 2.5 times;

- We found an increase of heat power of heat exchangers with intensifiers in the form of spherical or annular projections for a range of numbers Reynolds Re = 1200-3300 to 2.3-3 times in the flow of viscous fluids in tubes during the growth of the hydraulic resistance in the heat exchange tube system to 2,1-3,6 times.

3.2. The results are used to create a heat exchanger with heat power 65 kW and 26 kW for the cooling system EGR of gas engine KamAZ.

3.3. We have identified the impact of recirculation gases on emissions of harmful substances to exhaust gases and relative cost-effectiveness of the diesel engine fuel. The use of EGR system to reduce NOx emissions allowed by 28%.

3.4. We have proposed and numerically substantiated technical solution of significantly (1.5-time) increasing of the thermal efficiency of the condenser at the laminar heat transfer enhancement by elongated dimples.

Block 4 - Study of systems including heat exchangers and heat transfer processes:

4.1. On the basis of numerical simulations of air flow distribution inside the vehicle turbocharger, we analyzed the velocity and pressure distribution pattern in unsteady and steady air flow in the flow of the compressor. Based on these results we carried out impeller design optimization, the flow of the compressor, the cochlea. Due to this increased strength and stability of the dies

4.2. We have created a functional and mathematical models to calculate the temperature regimes and thermal processes occurring in the cooling elements and parts of piston engines, in which we have carried out numerical studies in the engine warming up. We have identified rational speed of water pump in the engine cooling system, allow you to reduce the engine warm-up and to provide its high technical and economic indicators. We proposed schematic and constructive solution of high-performance adaptive cooling piston diesel engine with controllable electrical drives the water pump. We have identified the optimal characteristics of the impeller of water pump. We have designed and manufactured high-efficiency impeller provide increased pressure by 30%, productivity by 15% and an efficiency of 20% at rated speed of the engine at speed of 3500 1/min.

4.3. To create a functional and mathematical models to calculate the temperature regimes and thermal processes occurring in the cooling system and the details of piston aircraft engines, which carried out numerical studies in the engine warm-up mode. The rational speed water pump in the engine cooling system, allow you to reduce the engine warm-up and to provide its high technical and economic indicators. Proposed schematic and design solution highly adaptive system cooling piston aircraft V-type diesel engine with regulated electric drive water pump, ensuring optimum thermal state of the internal combustion engine corresponding to the highest technical and economic, environmental and resource engine performance. The optimal characteristics of the impeller of water pump, designed and manufactured high-efficiency impeller provide increased pressure by 30%, supplying 15% and increase efficiency by 20% in nominal engine operation at 3500 1 / min.

4.4. We numerically investigated the heavy vehicle cabin ventilation and heating system. We conducted a study of heating and air conditioning control system. We upgraded elements of the cabin ventilation and heating system depending on the operating mode (shutter opening angle) by calculation results. We performed tests of the new system of ventilation and heating systems.

Shtork Sergey
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Advance modelling of physical processes in energy engineering and environment

SCIENTIFIC ORGANIZATION

Novosibirsk State University

ABSTRACT

The presentation will provide an overview of fulfilment results of the Lead Scientist Grant No. 11.G34.31.0046. This project has been targeted on establishing at Novosibirsk State University the Laboratory for Simulations of Processes in Energy Engineering. Main activities of the Laboratory were settled down on advanced theoretical, numerical (DNS, LES, advanced RANS and Hybrid methods) and experimental (laser based diagnostics – LDA, tomo- and stereo-PIV, LIF) studies of physical processes relevant to energy conversion, utilization and the environmental impact.

KEYWORDS

Hydropower Engineering, Combustion of Gaseous and Solid Fuels, Dispersion of Pollutants, Methane Gas Hydrates.

ACKNOWLEDGEMENTS

The work was financially supported by Lead Scientist (K. Hanjalic., NSU) Grant of RF Government No. 11.G34.31.0046 and Russian Science Foundation (RSF Grant No. 14-29-00203).

SUMMARY

The presentation contains some highlights and major achievements of fulfilment of the Lead Scientist (Prof. K. Hanjalic) Grant No. 11.G34.31.0046 (2011-2013, ext. 2014-2015). This project resulted in establishing the Laboratory for Simulations of Processes in Energy Engineering at Novosibirsk State University (NSU). The activities of the Laboratory cover the theoretical, computational and experimental investigation of turbulent single- and two-phase flows including chemically reacting (combusting) flows in various devices, equipment, machinery and installations used in modern energy conversion, storage and utilization technologies, as well as in chemical and mechanical engineering. The motivation is the optimization of performances and increase of efficiency of various energy engineering technologies and minimization of the man's impact on the environment and nature in general. In addition to gaining a deeper insight into the physics of various processes involved, the project has resulted in the development of new-generation computational codes for simulation and modeling of work processes in energy engineering as well as in the environment, which provide a tool for predicting performances and forecasting the ecological consequences of various technologies both in the planned (design) mode and in off-design and emergency modes.

The specific topics investigated include unsteady phenomena in hydropower engineering with focus on cavitation, related multi-phase phenomena and material erosion, vortical structures – vortex precessing and spiraling rope - in hydro-turbine draft tubes; combustion of gas- and solid fuels with focus on stabilization of low-emission lean flames by swirl and pulsation, extinction of diffusion flames over vaporizing liquids and solids, and combustion of mechanically-activated micronized coal; dispersion of pollutants in the atmosphere and water environment over complex terrain with heat islands, point and field pollution sources, under specific (and extreme) stratification conditions; evaporation, combustion and self-conservation of methane gas hydrates (the promising fuel of the XXI century).

Although the Megagrant has finished in 2015 the Laboratory continues working in these areas under financial support of the Russian Science Foundation grant (2014-2016, ext. 2017-2018).

ADDITIONAL INFORMATION

The presentation co-authors: Prof. Kemal Hanjalic, Prof. Dmitry Markovich.

Spaskova Elena
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Experimental studies of non-uniform displacement and strain fields at the complex study of the strength, vitality and destruction mechanisms reinforcing structural materials

SCIENTIFIC ORGANIZATION

Perm national research polytechnic university

ABSTRACT

The results of research of laws of accumulation of damage, destruction processes HIL coarse samples composite materials based on glass and carbon fiber reinforced plastics. Issues of determining the properties of load on the system, description of the data on the impact of characteristics of loading system on the kinetics of damage accumulation and the formation conditions macrodestruction composite products. The study of the damage accumulation laws HIL coarse samples composite materials based on glass-fiber-based application of the method of digital image correlation.

KEYWORDS

Non-uniform strain fields, digital image correlation, DIC, macrodestruction, coarse samples, composite products.

Temerova Marya
Researcher

Experimental studies of non-uniform fields of displacements and deformations during the quasi-static and dynamic tensile testing, punching, spinning the reinforcing fibers

SCIENTIFIC ORGANIZATION

Perm national research polytechnic university

ABSTRACT

The results of studies of the properties of the reinforcing fibers; an analysis of the mechanisms of deformation and destruction of samples of woven materials during the quasi-static and dynamic tensile testing, punching, drawing fibers using non-contact digital optical strain field analysis system.

KEYWORDS

Quasi-static testing, dynamic testing, tensile testing, punching, spinning, reinforcing fibers, DIC.

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Experimental and Theoretical Study of the Postcritical Deformation Stage of Materials Under the Various Types of Loading Conditions

SCIENTIFIC ORGANIZATION

Perm National Research Polytechnic University

ABSTRACT

The work is devoted to experimental study of the behavior of materials on the post-critical deformation stage at different types of the stress-strain state and loading conditions. Experimental and theoretical investigation of the postcritical deformation stage is necessary for forecasting of the behavior of materials in emergency cases and failure processes propagation. Results of uniaxial tension, proportional tension with torsion, complex tension-torsion loading and tension with additional vibrations are carried out.

KEYWORDS

Experimental mechanics, postcritical deformation stage, loading system, failure, survivability.

ACKNOWLEDGEMENTS

The work was carried out in the Perm National Research Polytechnic University with support of the Government of Russian Federation (The decree № 220 on April 9, 2010) under the Contract № 14.B25.310006, on June 24, 2013.

SUMMARY

Postcritical deformation stage of materials connected to the structural failure and fracturing processes and reflected on the strain curve as a descending section. Realization of the postcritical deformation stage allows using of the reserves of load-carrying ability, increase vitality and safety of the deformable systems. The work is devoted to experimental investigation of the behavior of structural carbon steels on the postcritical stage of deformation under different types of the stress-strain state.

The test results of uniaxial tension with various stiffness of the loading system with using of special test tool are obtained. It is demonstrate, that the failure moment of materials corresponds to a point on the descending section of strain curve and depends on stiffness of the loading system. Got results of the behavior of different structural steels on the postcritical stage of deformation under proportional and non-proportional tension-torsion tests at room and high temperature.

The methodic of realization of the additional vibrations during quasi-static tension with using of the biaxial test system is proposed. It is shown, that the additional loadings could lead to equilibrium deformation of specimen on the postcritical deformation stage.

ADDITIONAL INFORMATION

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SCIENTIFIC ORGANIZATION

Perm National Research Polytechnic University

The Spatial-Time Inhomogeneity of the Plastic Flow in Metals by Analysis of the Strain and Temperarure Fields

ABSTRACT

The work focused on the experimental study of the behavior patterns of the Al-Mg alloy and the carbon steel, in particular, the temporal instabilities and spatial localization due to the Lüder's behavior, the Portevin–Le Chatelier effect and the shoulder effect. The study based on the estimation of the inhomogeneous strain and temperature fields by use of the DIC technique and the IR analysis. The assessment of the influence of the loading conditions, the additional cyclic impact and the stress concentrators on the spatial-time inhomogeneity of the plastic flow was performed.

KEYWORDS

Jerky flow, the Portevin-Le Chatelier effect, the Luder's behavior, aluminum-magnesium alloy, digital image correlation, the IR analysis.

ACKNOWLEDGEMENTS

The work was carried out at the Perm National Research Polytechnic University with support of the Government of Russian Federation (The decree № 220 on April 9, 2010) under the Contract № 14.B25.310006, on June 24, 2013.

SUMMARY

The work focused on the complex experimental study of the behavior patterns of the Al-Mg alloy (Al — 2.2 %, Mg — 0.6 %, Mn — 0.4 %, Fe — 0.4 %, Si — 0.4 %) and the carbon steel (Fe — 99.0 %, C — 0.18%, Si — 0.20 %, Mn — 0.35 %, Cr — 0.04 %, Ni — 0.03 %, Cu — 0.04 %), in particular, the temporal instabilities and spatial localization due to the Lüder's behavior, the Portevin–Le Chatelier effect and the shoulder or necking effect. The aim of the study is to assess the influence of the loading conditions, the stress concentrators and the additional cyclic impact

on the effects of the serrated flow, on the initiation of the strain bands, and to interrelate local strain jumps with temperature bursts. The study based on the estimation of the inhomogeneous strain and temperature fields by use of the 3D digital image correlation measurement system Vic-3D and the infrared analysis system FLIR SC7600M. The mechanical tests were provided on the Instron 8850 servo-hydraulic biaxial testing system (100 kN/1000 N·m, 30 Hz) and the Instron 5989 electromechanical testing system (600 kN) at room temperature.

The research program included the following parts:

- the uniaxial tension of the flat dog-bone specimens with the constant rate of the kinematic loading from $0.33 \cdot 10^{-4}$ s^{-1} to 0.33×10^{-2} s^{-1} (steel);
- the uniaxial tension of the flat specimens with one and two holes with constant rate of the kinematic loading $1.67 \cdot 10^{-3}$ s^{-1} (steel);
- the uniaxial tension of the flat specimens with additional deformable parts and the flat specimens with complicated geometry with constant rate of the kinematic loading $1.67 \cdot 10^{-3}$ s^{-1} (Al-Mg alloy);
- the uniaxial tension with additional cyclic loading of the solid cylindrical specimens (steel).

For example, the σ–ε curve and the set of photos of the flat specimen during the Lüder's band nucleation (Fig. 1) and the evolution of the local strain rate and temperature fields on the surface of the flat specimen with two holes (Fig. 2) are illustrated below.

Fig. 1. Evolution of local strain rate fields at the stage of the yield plateau formation on the surface of the flat dog-bone specimen of the Al-Mg alloy

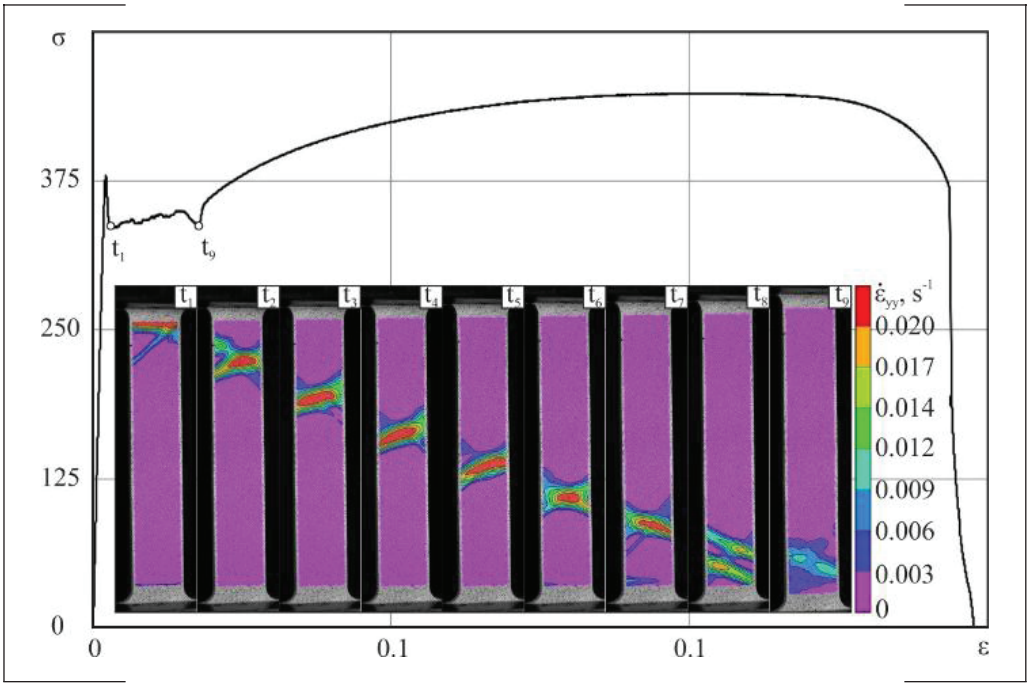
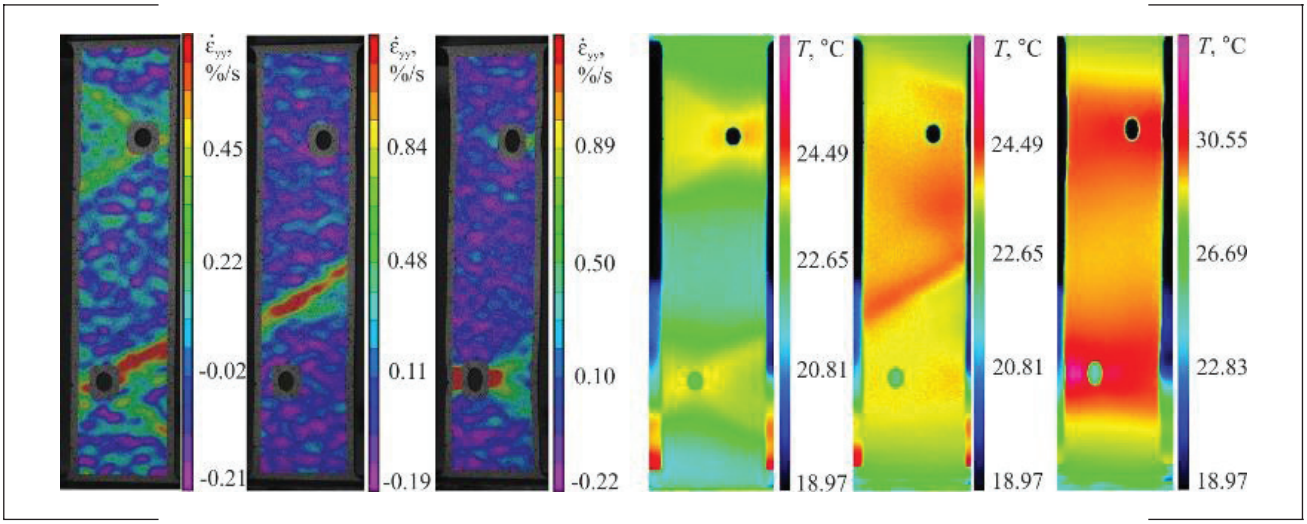


Fig. 2. Initiation and propagation of the strain bands on the surface of the flat specimen (the carbon steel) with two holes.



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Electrochemical devices based on solid oxide proton-conducting electrolytes: a review

SCIENTIFIC ORGANIZATION

University of Thessaly

ABSTRACT

The present review work is devoted to the research achievements obtained the last two years in the Megagrant laboratory of electrochemical devices based on solid oxide proton-conducting electrolytes at the Institute of High Temperature Electrochemistry in Ekaterinburg. In the last 2 years more than twenty works have been published in International journals. These works are devoted to: i) design and development of new proton conducting solid electrolytes and electrodes, ii) amperometric and potentiometric gas sensors, iii) electrolyzers for hydrogen production.

KEYWORDS

Solid oxide conductors, protonic electrolytes, solid oxide fuel cells, electrolyzers, sensors, electrochemical reactors.

ACKNOWLEDGEMENTS

Authors are grateful to the Ministry of Education and Science of the Russian Federation (contract no. 14.Z50.31.0001) for the financial support.

SUMMARY

The research history in the field of protonic electrolytes is reflected in literature [1-2]. The theoretical and practical aspects, emphasizing the general principles and guidelines necessary for the design and development of future electrochemical systems based on solid oxide proton conducting electrolytes (fuel cells, electrolyzers, gas sensors, reactors), are studied in the new laboratory and part of the results is thoroughly presented and discussed in the already published works [3-4].

High-temperature proton-conducting materials are widely proposed as electrolytes for applications in electrochemical devices, including solid oxide fuel cells (SOFCs), electrolyzes, sensors, hydrogen-permeable membranes for hydrogen production or ammonia synthesis [3].

Having previous experience in related solid state electrochemistry topics, the last two years our main research work has been focused:

1. On the detailed analysis of thermal and chemical compatibility of cathode materials for $BaCeO_3$ and $BaZrO_3$-based electrolytes for solid oxide fuel cell application [4-6].

In this research work the identification of suitable cathode materials, which can be successfully used in SOFCs based on proton-conducting electrolytes during long-term operation and thermal cycling measurements was investigated. In order to better be informed about, a wide variety of materials were synthesized and their thermal and chemical compatibilities toward $BaCe_{0.8}Y_{0.2}O_{3-\delta}$ and $BaZr_{0.8}Y_{0.2}O_{3-\delta}$ were verified by means of detailed dilatometry and XRD analysis of calcined electrode/electrolyte mixtures, respectively. It was found that some of the studied cathode materials react to a different degree with selected electrolytes. The main attention was paid to the comparison of thermal behaviours of cathode and electrolyte system as well as the chemical compatibility between them.

Taking into account the relatively low TEC values, no significant chemical expansion and high resistance to impurity phase formation, $LaNi_{0.6}Fe_{0.4}O_{3-\delta}$ and $La_2NiO_{4+\delta}$ samples can be proposed as suitable cathodes for $BaCe_{0.8}Y_{0.2}O_{3-\delta}$ and $BaZr_{0.8}Y_{0.2}O_{3-\delta}$ electrolytes. The layered $Y_{0.8}Ca_{0.2}BaCo_4O_{7+\delta}$ cobaltite has the closest TEC value with those for cerate and zirconate ceramics, however completely decomposes after treatment of $Y_{0.8}Ca_{0.2}BaCo_4O_{7+\delta}/BaCe_{0.8}Y_{0.2}O_{3-\delta}$ mixture and was stable in contact with $BaZr_{0.8}Y_{0.2}O_{3-\delta}$.

2. On the design and development of appropriate proton conducting electrolytes and electrode materials for possible application in solid oxide fuel cells and solid oxide electrolyzers [7-8].

To this aim the relationship between Y by Yb substitution on the crystal and microstructure properties as well as thermomechanical and electrical features

of $BaCe_{0.5}Zr_{0.3}Y_{0.2-x}Yb_xO_{3-\delta}$-based ceramics ($BCZYYb_x$) was investigated. It was shown that the increase of Yb concentration from 0 to 0.2 leaded to decrease of: i) the unit cell parameters/volume (from 490.57 to 486.80 Å^3), ii) the TEC values (from $8.5\cdot10^{-6}$ to $7.6\cdot10^{-6}$ K^{-1}). However, the concentration dependences of mean grain size and total conductivity of $BCZYYb_x$ ceramics were similar, fact that allows one to conclude that the grain boundary significantly affects the transport properties of these proton-conducting electrolytes.

Moreover we demonstrated that a tape calendering method (TCM) is an effective way for the preparation of proton ceramic fuel cells with enhanced performance. More precisely the possibility of proton ceramic fuel cell (PCFC) fabrication, using TCM, has been shown for first time for $Ba(Ce,Zr)O_3$-based proton-conducting electrolytes.

The as fabricated cell consisted of a 30 μm $BaCe_{0.5}Zr_{0.3}Y_{0.2}O_{3-\delta}$ (BCZY) electrolyte, a $Y_{0.8}Ca_{0.2}BaCo_4O_{7+\delta}$ cathode and the reduced 40%BCZY + 60%NiO and 45%BCZY + 55%NiO support and functional anode layers. Phase structure, thermal and electrical characterization of functional materials were also discussed in detail. It was found that the maximal power densities (P_{max}) of the fabricated PCFC (174 and 308 mW cm^{-2} at 600 and 725 °C, respectively) were acceptable for an intermediate-temperature range of operation and comparable with those reported in literature. The BCZY electrolyte exhibited very high open circuit voltage (OCV) values (1.141 and 1.079 V at 600 and 725 °C) and, correspondingly, predominant ionic transport (average ions transport number 0.99 and 0.95 at 600 and 725 °C).

In our opinion, the tape calendering method can be considered as effective strategy for PCFCs fabrication, ensuring the formation of gas-tight electrolytes and acceptable electrochemical properties.

3. On the sulfur and carbon tolerance of BaCeO3–BaZrO3 proton-conducting materials [9].

For this purpose, $BaCe_{0.8-x}Zr_xY_{0.2}O_{3-\delta}$-based ceramic samples ($BCZY_x$) were prepared and their chemical stability in corrosive atmospheres containing high concentrations of H_2O, CO_2 and H_2S was investigated. Based on both the fresh (not exposed) and the treated (exposed to corrosive atmospheres) samples, the estimation of the tolerance degree was obtained by determining the: i) phase structures, ii) unit cell parameters, iii) surface microstructures, and iv) electrical conductivities.

Fresh ceramics were found to be single-phased in the whole range of *x* and all the treated materials exhibited good chemical stability in the water vapor atmosphere, whereas the samples with $0 \le x \le 0.2$ and $0 \le x \le 0.3$ were not single-phased in pure CO_2 and 10% H_2S/Ar, respectively. The analysis of crystal structure and transport characteristics of the treated $BCZY_{0.3}$ samples has shown a weak deviation of unit cell parameters and no degradation in electrical conductivity. For fresh $BCZY_{0.3}$ the transport nature in various atmospheres was also evaluated. At 600 °C the $BCZY_{0.3}$ exhibited conductivity of 2.7, 4.0, 1.7 and 3.7 mS cm^{-1} in air, wet air, hydrogen and wet hydrogen atmospheres, respectively. Based on the obtained results, $BCZY_{0.3}$ can be considered as a perspective proton-conducting material having reasonable transport and tolerance properties.

4. On the design and development of potentiometric and amperometric sensors for gaseous components determination [10-12].

The potential application of $BaCe_{0.7}Zr_{0.1}Y_{0.2}O_{3-\delta}$ proton-conducting material as an electrolyte for hydrogen sensor operating under potentiometric and amperometric modes was also investigated. The reason of selection of $BaCe_{0.7}Zr_{0.1}Y_{0.2}O_{3-\delta}$ composition was caused by optimal combination of target properties, including acceptable stability and thermal properties of the material as well as high proton conductivity. The dense electrolyte materials were used as a base of the electrochemical cells of the sensor and then sensor's electrochemical properties were measured under different H_2-containing atmospheres and temperatures. The obtained results demonstrate the response of the hydrogen sensor in both modes of operation. Its operability was confirmed by comparing the experimental data with theoretical predictions. The sensor based on the $BaCe_{0.7}Zr_{0.1}Y_{0.2}O_{3-\delta}$ proton-conducting electrolyte can be successfully used for the detection of hydrogen content (0.1–10 vol.%) in nitrogen at the temperature range between 450 and 550 °C.

5. On the utilization of proton conducting materials in electrochemical reaction (mostly reductions of CO_2 for methanol production and of N_2 for ammonia synthesis) [13].

In order to provide information about the possibility of using proton electrolytes in electrochemical reactions for carbon dioxide of nitrogen hydrogenation (for methanol or ammonia preparation respectively), the steady-state current-overpotential characteristics of the Fe|$BaCe_{0.5}Zr_{0.3}Y_{0.08}Yb_{0.08}Cu_{0.04}O_{3-\delta}$|Fe interface as a function of the gas phase composition and temperature were investigated.

To this purpose a $BaCe_{0.5}Zr_{0.3}Y_{0.08}Yb_{0.08}Cu_{0.04}O_{3-\delta}$ material is successfully synthesized by solid state synthesis and sintered to dense ceramics at 1400 °C. Then its crystal structure, ceramic and electrical properties are investigated. It was found that the ceramic had a high relative density (more than 90%) and acceptable proton conductivity (1.5 and 6.8 mS cm^{-1} at 500 and 900 °C, respectively). On the as prepared $BaCe_{0.5}Zr_{0.3}Y_{0.08}Yb_{0.08}Cu_{0.04}O_{3-\delta}$ electrolyte disk, three thin Fe porous layers were deposited by painting on both sides (three electrode system), which was then immersed in a tubular single-chamber continuous electrochemical reactor.

The polarization measurements were carried out in the temperature range between 500 and 700 °C and at three different H_2/He wet (3% steam) compositions. The apparent anodic and cathodic charge transfer coefficients (Tafel region) are found to be: $\alpha_a = \alpha_c = 0.8$, while the apparent activation energy was calculated to be approximately 0.55 ± 0.05 eV. It was also found that by increasing the hydrogen concentration the current density increases, especially at higher temperature value.

6. On the comparative analysis of various synthesis methods for the preparation of Proton-conducting electrolytes based on Ba(Ce, Zr)O_3 [14]

The identifying possible synthesis ways for the formation of a proton-conducting electrolyte based on $BaCeO_3$ and $BaZrO_3$ solid solutions has also been thoroughly investigated in the frame of our MG project. Among different methods (solid-state reaction, citrate-nitrate combustion, oxalate co-precipitation) and their CuO-modified analogs, the citrate-nitrate combustion or solid-state reaction synthesis coupled with the introduction of 0.5 wt% CuO were found to be more appropriate strategies for the development of not only single-phase, but also high-dense $BaCe_{0.5}Zr_{0.3}Y_{0.2}O_{3-\delta}$ ceramics.

The XRD and SEM analysis, dilatometry method and hydrostatic weighing were used for the estimation of quality of ceramics. The results obtained demonstrate that the use of SSR and CNC methods modified by the introduction of 0.5 wt% CuO promotes the achievement of the necessary properties of ceramic samples (excellent densification, single-phase, and non-porous microstructure).

The research activity of our research group is still continuing this year with the fabrication of prototypes of solid oxide fuel cells, solid oxide electrolyzers and amperometric/potentiometric sensors, using the as developed proton conducting materials.

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SCIENTIFIC ORGANIZATION

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Experimental study of the low-cyclic fatigue under variable parameters of cycle at various temperatures and types of loading

ABSTRACT

The work is devoted to experimental study of the low-cyclic fatigue of structural steels and aluminum alloys under variable parameters of cycle. Test results of uni-axial tension-compression, proportional and complex tension with torsion at room and high temperature are obtained in the project.

KEYWORDS

Low-cyclic fatugue, tension, tension-torsion, complex loading.

ACKNOWLEDGEMENTS

The work was carried out in the Perm National Research Polytechnic University with support of the Government of Russian Federation (The decree № 220 on April 9, 2010) under the Contract № 14.B25.310006, on June 24, 2013.

SUMMARY

Uniaxial tension tests were carried out on Instron 8801 servohydraulic test system (maximum load of tension and compression is 100 kN, cyclic tests with frequency up to 30 Hz) with using of axial extensometer Instron 2620-601. Biaxial tension-torsion tests were carried out on Instron 8850 biaxial servohydraulic test system (maximum load of tension and compression is 100 kN, maximum torque is 1000 Nm, cyclic tests with frequency up to 30 Hz) with using of biaxial (tension with torsion) extensometer Epsilon 3550-010M and Epsilon 3550HT-025M.

In tests were used solid cylindrical and thin-walled tubular specimens of structural steels and aluminum alloy. Triangle and M-shape cycles and block loading were realized in the uniaxial and biaxial tests. In the complex tests under tension and torsion, the trajectories with bend in axis of axial strain and shear angle were used.

ADDITIONAL INFORMATION

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Transition Prediction Methods for Aerodynamic Flows.

SPECIAL SESSION

"Development of international scientific cooperation in research and development in priority areas of science and technology"

Abstract. In this paper, the potential of transition prediction methods is explored for modelling transitional shock-wave/boundary-layer interactions. The study is fuelled by the strong interest of researchers and airframe manufacturers in reducing drag of vehicles flying at transonic speeds. The principle of drag reduction via flow laminarity is valid, provided there is no need for the flow to sustain large pressure gradients or shocks. This is true since laminar boundary layers are less resistant to flow separation. At this work, the CFD solver of Liverpool University is used. The results suggest that the intermittency based model captures the fundamental physics of the interaction but verification and validation is needed to ensure that accurate results can be obtained. Summary: This paper presents the development and application of transport-based transition models for CFD. Two challenging problems are addressed including flow at low Mach and high Reynolds numbers as well as problems at high transonic Mach and moderate Reynolds numbers. The work suggests that with proper calibration this family of models can provide results with good engineering accuracy. Keywords: CFD, Transition modelling Acknowledgment: Part of this work was supported by the EU F7 TFAST project.

Camussi Roberto

Roma Tre, Italy

Opportunities for University Roma Tre and CIRA's participation in joint youth research projects, possible research areas.

SPECIAL SESSION

«Development of international scientific cooperation in research and development in priority areas of science and technology»

The presentation will describe possible topics of interest for developing future collaborations between Italian and Russian young scientists in aeroacustics. In the first part of the talk, a description of the Roma Tre institution as well as of the research groups active therein in the aeroacoustic field will be given. In the second part, a description of a few research theme of specific interest will be provided with special emphasis to experimental activities including jet noise applications and advanced post -processing techniques. The contribution of CIRA (Italian Aerospace Research Center) will be also outlined and topics in aeroacoustic of interest for this research centre will be briefly discussed.

Dutov A.V.

FSBI "National Research Center "Institute named after N.E. Zhukovsky"

Intersectoral integration as a source of technological development of aircraft engineering and other high-technology industries: priorities and opportunities for international cooperation.

SPECIAL SESSION

«Development of international scientific cooperation in research and development in priority areas of science and technology»

The global challenges the aviation in the world faces enforce making technological breakthroughs pointed to multiple increase of aviation mobility while maintaining an acceptable level of safety and environmental impact of air transport. Thus, the aircraft of the future must meet strict, often conflicting requirements. Russian aircraft industry is facing specific national challenges, in addition to global challenges mentioned above. They include making air transport available to the citizens and maintaining transport connectivity of the country, including sparsely populated regions with hard climate conditions. Entrance into the global civil aviation markets requires not just a parity level of Russian aircraft industry products, but their «breakthrough» advantage over the products of competitors.

At the same time, opportunities for research and technological development of aviation in the traditional areas and destinations are close to exhaustion. Technological breakthroughs are possible in the field of intersectoral technology integration, the collaborative development of technologies that benefit multiple

industries. Economic rationales for such integrative strategy are obvious. The consolidation of efforts, competences, ideas and resources and the elimination of wasteful research and development work and experimental base overlapping allows to achieve the desired results in a shorter time, with lower risks. In addition, expenditures on research and development made while creating new technologies will be later distributed on the entire production volume of several industries, including those having larger production volumes compared to the aircraft industry.

So, the following directions of research and development aimed at creating breakthrough technologies for both aircraft and other high-tech industries can be outlined. According to the main strategic documents determining the development areas of science and technology in the aviation industry, priorities of civil aviation development are:

- increasing the availability and quality of air transport services;
- ensuring the acceptable level of flight safety and security;
- reducing the harmful impact of aviation on the environment.

It is noteworthy that similar problems are relevant for a number of high-tech industries, including cars or ships manufacturing, power engineering etc. Accordingly, the opportunities for intersectoral technology integration can be identified in the areas of:

- new energy sources, its storage and conversion on board;
- new structural materials, constructions and manufacturing technologies;
- methods and tools for automation of the moving objects and complex systems control, including those based on the principles of artificial intelligence;
- new methods of mathematical modeling, calculation and design of complex systems.

The directions of intersectoral technology integration can be classified according to the following criteria:

- the industry which receives aviation technologies;
- the sector or subsector which is the source of aviation technologies (aircraft construction, propulsion engineering, instrument engineering, etc.);
- the disciplines or areas of basic research, that are involved in creating the necessary fundamental advance – for example, life sciences, information sciences, fundamental physics and chemistry, socio-humanities, etc.;
- life cycle stage on which the intersectoral integration is conducted: the common technologies may apply to the field of research methods and tools, to the product development and design, or these may be the technologies already embodied in specific products and principles of their operation.

The report gives examples of these categories of science and technology intersectoral integration areas for aviation and other high-tech industries, as well as examples of international cooperation in these areas, or the potential for such cooperation. They are identified using the methodology of strategic planning of inter-industry integration of technologies developed by National research center «Institute named after N. E. Zhukovsky». The main idea of this approach is that the desired values of future prototype characteristics are determined based on the system of goals expressed in quantitative form. Using a system of models for estimating technology impact on these integral characteristics, we can evaluate if the target values can be achieved by means of:

- the known technologies, traditionally used in the industry or technical field;
- the technological solutions new for the industry or technical field, new fundamental scientific results, etc.

Special attention while evaluating the effectiveness of intersectoral integration of new technologies is paid on the assessment of technological similarity of various industries participating in the integrated scientific and technological projects. The degree of technological similarity influences the optimal choice of participant sectors. Optimality here means ensuring maximum applicability of the created scientific and technological potential for various industries, as well as the possibility of creating breakthrough technologies in a short time with an acceptable level of risk.

Kan Anna V.

Main areas of international cooperation in the development of advanced avionics systems FSUE «GosNIIAS».

SPECIAL SESSION

«Development of international scientific cooperation in research and development in priority areas of science and technology»

Over the past several years FGUP “GosNIIAS” has been a major player in scientific and research activities under the frames of “Development of Russian civil aviation engineering in 2002-2010 and until 2015” federal target program and “Development of Aviation Industry in 2013-2015” national program.

One of the main directions of these scientific and research activities is development of process automation technologies related to design of certified aircraft avionics based on integrated modular avionics (IMA). This topic is especially important due to expansion of international cooperation of scientific and instrument-engineering companies.

The character of international cooperation requires a special attention to formalization of the basis of design requirements, to the purchase equipment as well as to designed production, to specification documents and to the production and service quality control and analysis.

Several European R&D projects within Frameworks 6 and 7 by EC were dedicated to this issue. One of the topics of Horizon 2020 was focused on design of unified set of software tools to support IMA-based avionics development and certification. Results of these studies were applied in A-380 and Superjet100 designs.

Different companies have different sets of software tools approved by certification authorities during certification of avionic complexes based on federated principle. But at the same time the most successful specific items became commercial products. At this stage a business competition grew up and the tools perfection played more important role which caused reduction of strict requirements given by customers.

At the moment there are many software tools providing support of life cycle processes for avionics and some of them create a tendency for future development. It is possible to specify: Requirements management tool based on IBM technologies, SCADE visual programming tools that are providing an automatic generation of certified code and Wind River Workbench integrated coding environment.

Foreign companies are actively using the software tools providing avionics life cycle support. This type of software usually has a central position in production design as well as it builds a base for further avionics certification. Russian companies don’t have experience in avionics design and certification in frames of such process approach.

That is why the idea of application of the process approach in aviation instrument-engineering companies is important. It should be applied in the process of the software design, which should meet DO-178B requirements and be supported by specified tools that are providing process automation on every stage of the software life cycle.

Based on the best approach given by foreign certification authorities, in the frame of this R&D, there was created a special source environment, which is supporting a life cycle of IMA-based avionics design.

At the moment these tools are on the stage of prototype testing in aviation companies. Further activities include development of ISO 15288-2008 based Russian platform supporting different system engineering processes on different stages of the life cycle of IMA-based avionics design.

Kopiev V.F.

FSUE "Central Aerohydrodynamic Institute named after prof. N.E. Zhukovsky (TsAGI)"

Experience of leading scientists and universities' interaction in the framework of the Resolution No.220 of MES, possibilities of participation of new laboratories in joint projects.

SPECIAL SESSION

«Development of international scientific cooperation in research and development in priority areas of science and technology»

In the laboratory established under the Resolution No.220, contract No.14. Z50.31.0032, it is possible to carry out the following works:

(i) in the new anechoic chamber to carry out studies of noise from a single-circuit turbulent jet and vortex rings;

(ii) by the azimuthal decomposition method (ADM) with a reduced number of microphones, to carry out tests of a full-scale jet on an open stand;

(iii) apply noise source localization techniques (beamforming) to real engines;

(iv) To investigate the modal structure of sound field in a full-scale air inlet in the anechoic chamber and at the full-scale stand;

(v) to use sound absorbing structures impedance extraction methods for engine channels and sound absorbing structure manufacturing;

These activities could complement TsAGI's works in this direction in the framework of both contracts with the Ministry of Industry and Trade and Ministry of Education and Science of the Russian Federation and contracts with such enterprises as Aviadvigatel JSC, Irkut Corporation, Sukhoi Civil Aircraft Company and others.

Kopiev V.F.[1,2], Palchikovskiy V.V.[1], Belyaev I.V.[1,2], Bersenev Yu.V.[1], Makashov S.Yu.[2], Zaitsev M.Yu.[1,2], Khramtsov I.V.[1], Kustov O.Yu.[1], Korin I.A.[1], Sorokin E.V.[1]

1 Perm National Research Polytechnic University, Perm, Russia

2 Central Aerohydrodynamic Institute, Moscow, Russia

New anechoic chamber for aeroacoustic research: development, qualification tests, use in experiments.

SPECIAL SESSION

«Development of international scientific cooperation in research and development in priority areas of science and technology»

Principal stages of development and use in aeroacoustic research a new anechoic chamber built in Perm National Research Polytechnic University (PNRPU) in 2014-2015 are presented. It is shown some design features of the anechoic chamber. The qualification tests have determined that the anechoic chamber in PNRPU realizes the free-field conditions. The radius of the region where the inverse square law spreading is observed equals to 3 m in the frequency range 125 Hz – 20 kHz, provided that microphones are at least at the distance of 1 m from the wedge tips.

To carry out in the chamber research involving noise generation by aerodynamic sources the jet rig and vortex ring generator were designed and built. The jet rig reaches velocity equal to 200 m/s with nozzle exit diameter of 8 cm. The measurements in the PNRPU anechoic chamber have shown that spectra of turbulent jet noise are the same trends as those of known jet rigs. The experiments carried out in the anechoic chamber revealed that vortex ring noise can be determined on initial path of vortex ring motion even at background noise of the generator. In spectrum there is a peak of acoustical pressure, which is typical of vortex ring. Subsequent motion of the vortex ring leads to shift this peak in lower frequencies. Observed effects are in good according to those obtained earlier in anechoic chamber AC-2 TsAGI.

Thus, experimental results demonstrate that the anechoic chamber allows the aeroacoustic measurements to be performed to obtain quantitative results. In addition, one can say that designing and building PNRPU anechoic chamber led to restore of domestic capacities in the development and production of acoustical wedges.

The work has been performed with the financial support of the Russian government under grant "Measures to Attract Leading Scientists to Russian Educational Institutions" (contract No. 14.Z50.31.0032).

Kustov O.Yu.,
Lapin I.N.,
Palchikovskiy V.V.

Perm National Research Polytechnic University, Perm, Russia

Peculiarity of experimental research of sound-absorbing liner specimens produced by 3d printing.

SPECIAL SESSION

«Development of international scientific cooperation in research and development in priority areas of science and technology»

Using 3D printing to create liner specimens is the only way at present to test in experiments the liner patterns with new-designed resonator geometry, because standard technologies of liner production provide liners with only simple resonators. However, identity of acoustical properties of liners produced from standard materials (composites, aluminium) and 3D printing materials is a free-answer question.

To carry out comparative tests the liner specimens with two different cell sizes and porosity of perforated plates of 5, 7 and 11 % were produced by 3D printing from ABS plastic. These specimens were compared with those made of glass-fibre plastic and aluminum. Compared specimens have absolutely the same hole arrangements and perforated plate porosity (there was 24 variants in all). Experiments were carried out in impedance tube with normal incident waves in the frequency range 500-6400 Hz at sound pressure level 140 dB.

Obtained data have shown that sound absorption coefficient of the liner specimens produced by 3D printing from ABS plastic, can be differ by 0.2 from those of standard material liners, which is considerably. In addition, resonant frequencies are also differ. Thus, one can conclude that production of new liners by 3D printing can be used in experimental research of acoustic properties of the new resonator geometry, but consideration must be given to the fact, that properties of the produced liner specimens would be different from those produced by standard technology and with other materials. It is necessary to carefully select the 3D printer to produce liner specimens.

The work has been performed with the financial support of the Russian government under grant "Measures to Attract Leading Scientists to Russian Educational Institutions" (contract No. 14.Z50.31.0032).

Lanshin A.I.

Doctor of engineering

FSUE "Baranov Central Aircraft Engine Institute (CIAM)", Russia

International cooperation in perspective aviation and aerospace power unit research.

SPECIAL SESSION

«Development of international scientific cooperation in research and development in priority areas of science and technology»

International cooperation of the Baranov Central Aircraft Engine Institute began since its foundation in 1930. The cooperation areas have been changing along with the development of aviation and space technologies.

Currently these cooperation areas cover whole spectrum of scientific and technical activities of CIAM: from the research of alternative fuels and reciprocating engines to high-speed power units of perspective reusable space transportation systems. This research focuses on the problems of the development of gas turbine propulsion and auxiliary engines.

The Institute is involved as a partner in international integrated projects of the 7th and 8th Framework program of the European Union, a partner of the European Commission-funded projects ESPOSA, LEMCOTEC and ENOVAL. In addition, CIAM participates in the implementation of cooperation projects COBRA, HEXAFY-INT and AGILE.

Within the framework of bilateral cooperation The Institute has long-standing relationships with all leading engine manufacturing companies and research centers in Europe, such as DLR, ONERA, ESA, SAFRAN Group, Airbus Group, MTU Aero, Avio aero, Rolls-Royce and many others. In addition, the Institute continues to work with its traditional partners from the CIS. In the east, the Institute carries out research work for the People's Republic of China and the Republic of India.

CIAM is involved in several international scientific societies: ISABE (International Society for the jet engine), ICAO, ICAS, ASME, AIAA, SAE and others, as well as in

international forums, including the MAKS (Russia), Le Bourget (France), Farnborough (UK), the ILA (Germany), the exhibition “Engine” (Russia), AIRCHINA (China), Airshow India (Bangalore), and others.

CIAM develops international cooperation in solving urgent problems of aviation and aerospace power unit development in the following research areas: aerodynamics, heat transfer, acoustics, emissions of harmful substances, burning, durability and reliability, processes and mechanisms of icing, the use of fuel cells in aviation technology, “electrical technology “aircraft, multidisciplinary optimization of perspective aircraft power units, alternative aviation fuels and others.

Sukhanov V.L.

FSUE “Central Aerohydrodynamic Institute named after prof. N.E. Zhukovsky (TsAGI)”

Interaction of Russian and foreign scientists in the framework of international programs.

SPECIAL SESSION

«Development of international scientific cooperation in research and development in priority areas of science and technology»

1. State support of international cooperation in the field of aeronautics

- To maintain the competitiveness of the Russian aviation industry and to strengthen its position at the world market the Government of the Russian Federation provides substantial assistance via respective and effective government programs
- The Ministry of Industry and Trade of Russia develops international cooperation with the aim of developing a global service network and completing the aviation industry reorganization.
- The Ministry of Education and Science of the Russian Federation contributes significantly to the creation of a competitive and efficient applied research and development sector. The Federal Target Program “Research and development in priority areas of Russian scientific and technological complex for 2014-2020”, set for the period until 2020, aims to support the creation of products and technologies for the modernization of the economy in priority areas, to implement a quality solution of new scientific and technological problems and to integrate the Russian research and development sector into the global innovation system.
- Significant support for the development of international relations is on the part of the The Federal Agency for the Commonwealth of Independent States, Compatriots Living Abroad and International Humanitarian Cooperation (Rossotrudnichestvo) as the Federal Agency for International Cooperation, which adheres to the federal strategy for the organization of short study visits to Russia for foreign representatives of political, social and scientific institutions. RSF Russian Science Foundation -provides financial and organizational support of fundamental research, education, development of research groups which occupy leading positions in various fields of science.
- In 2014, the President of the Russian Federation approved the establishment of the National Scientific Center “Institute named N.E. Zhukovsky”, which consisted of five organizations: FSUE “TsAGI “, FSUE “Baranov Central Aircraft Engine Institute (CIAM)”, FSUE “GosNIIAS”, FSUE “Siberian Aeronautical Research Institute named after S.A. Chaplygin” and FFE “GkNIPAS”. The National Research Center aims at strengthening the state influence on the development of aviation science, creating competitive aircraft models and using advanced technologies for further economic growth of the country.

2. Cooperation with the European countries in the field of aeronautics

- The Russian Federation pays special attention to the strengthening of international cooperation, in particular, activity of the Russia-EU working group established in 2007 and the National Contact Point for Aeronautics (NCP) which operates on the basis of FSUE “TsAGI” since 2004 with the purpose of informing, consulting and providing methodological support for cooperation between Russian and European research organizations.
- The main objectives of the NCP representation office in Brussels are the development and strengthening of international scientific and technological cooperation in the field of aeronautics between Russian and European partners. TsAGI, acting as NCP, is involved in the following associations: EREA (Associate Member of the

Association of European Research Establishments in Aeronautics), CEAS (admitted to the Council of European Aerospace Societies), EASN (Member of the European Aeronautics Science Network) and ETNA Plus (Associate member of the European Transport Network Alliance project). Besides, TsAGI acts as the coordination center of the X-Noise project in Russia (Coordination and Research Network in the field of aircraft noise).

3. Russia's activities in the framework of international programs

- Russian aviation sector organizations have implemented and continue to implement more than 50 joint research projects with partners from the EU in the framework of the 6th, 7th framework programs as well as under the "Horizon

Figure 1. Joint projects with EU partners

- As part of the 7th Framework Programme there are carried out research projects such as HEXAFLY-INT (High-Speed Experimental Fly Vehicles – International), PolarBear (Production and Analysis Evolution For Lattice Related Barrel Elements Under Operations With Advanced Robustness), RESEARCH (RELIABILITY AND SAFETY ENHANCED ELECTRICAL ACTUATION SYSTEM ARCHITECTURES), Buterfli (BUffet and Transition delay control investigated within European-Russian cooperation for improved FLIght performance).
- In the framework of the «Horizon 2020» program Russia is actively involved in such projects as AGILE (Aircraft 3rd Generation MDO for Innovative Collaboration of Heterogeneous Teams of Experts), Tilda (Towards Industrial LES/DNS in Aeronautics — Paving the Way for Future Accurate Computational Fluid Dynamics), Future Sky Safety in the framework of the «Future Sky» program and the ASPIRE project (Aerodynamic and acouStic for high-by-Pass ratIo tuRbofan intEgration) in the framework of the «Clean sky 2» program.
- International cooperation is actively developing in the framework of European national programs: Lifting off (UK), Take off (Austria), European national programs within the DASR cluster (Netherlands).
- International scientific seminars, such as TsAGI-DLR (German Aerospace Research Centre) and TsAGI-ONERA (French National Aerospace Research Centre), are held yearly and play an important role in the long-term consolidation of the major aviation centers. The seminars provide an opportunity to present research activities in the field of aeronautics for both leading scientists and young professionals. Sharing research results and the common interest in conducting scientific experiments stimulate the development of new projects and the promotion of advanced technologies.
- In addition, TsAGI actively participates and is one of the organizers of ICAS (International Council of Aeronautical Sciences) and IFASD (International Forum on Aeroelasticity and Structural Dynamics) forums.

Sypalo Kirill

Doctor of engineering, Professor of the Russian Academy of Sciences

First Deputy Director of the National Research Center "Institute named after N.E. Zhukovsky"

Interdisciplinary integrated projects in the aviation industry.

SPECIAL SESSION

«Development of international scientific cooperation in research and development in priority areas of science and technology»

Process safety and independence of our country in the current geo-political and economic conditions require a new look at the control system of the technological advance establishment, as the basis of formation of competitive high-tech industry and economy. Along with the optimization of the priority directions of scientific and technological development of Russia and the concentration of resources in these areas one of the most important principles of modern science is the research and development at the interface of disciplines and industries, which is a necessary condition for the creation of breakthrough technologies, as in most sectors of the knowledge-based industry the possibilities of achieving technological breakthroughs in isolated scientific fields have been exhausted.

An instrument for creating breakthrough technologies may include:

-In basic science -the convergence of disciplines -the creation of new disciplines at the intersection of the existing ones.

-In applied science -interdisciplinary integration -the creation of new technologies with the use of methods and means of the various disciplines. The technologies of synthesized and integrated vision in aviation can be used as an example.

Nowadays integrated scientific and technological projects on the basis of system integration of technology which are the "Foundation" of the subprogram "Aviation Science and Technology" in the state program of Russian Federation "Development of the aviation industry in the years of 2013-2025." are instruments of such integration. Complex scientific and technological projects combine the complex of research projects in order to finalize the selected technologies, which were generated in the process of fundamental research and which have reached level 2-3 of technology readiness (TRL), based on the system integration methods, ensuring mutual coordination and optimal integration of emerging technologies in the framework of the target system formation (aircraft, aircraft engine, system or machine), as well as the integration of new technologies in the framework of the main stages of aircraft life cycle (production, operation, utilization).

Such scheme allows an optimal way to implement the applied "bind" of the research results to the industry, to develop a science-based technological forecasts and comprehensive plans for the development of technologies that really get breakthrough results at the intersection of disciplines and the possibility of scientific and technological potential in many sectors of the knowledge-based industry.

MATHEMATICS & MECHANICS

Akhatov Iskander

Doctor of Physical and Mathematical Sciences

Professor and Director of the Center for Design, Manufacturing and Materials

SCIENTIFIC ORGANIZATION

Skolkovo Institute of Science and Technology

Multiphase Fluid Dynamics of Materials Deposition

ABSTRACT

In the paper mathematical models, numerical algorithms, experimental studies and practical applications of Aerosol Beam and Cold Spray Direct-Write processes will be presented.

KEYWORDS

Micro-fluidics, aerosols, droplets, Saffman forc.

ACKNOWLEDGEMENTS

This study is supported in part by Grant of Ministry of Education and Science of the Russian Federation (11.G34.31.0040) and Skoltech Partnership Program.

SUMMARY

The advent of new emerging technologies in materials deposition during recent years, along with new experimental tools, as well as substantial progress in high performance computing, have resulted in a growing research thrust directed to understanding of the nature of the high speed multiphase flows in micro-scale. In this paper, two types of so-called “direct write” processes will be discussed from theoretical and experimental viewpoints.

Aerosol Beam Direct-Write. It is shown that under proper conditions an aerosol flow through micro-capillary reveals new manifestation of microfluidics: the Saffman force acting on aerosol particles in gas flowing through a micro-capillary becomes significant thereby causing noticeable migration of particles toward the centerline of the capillary. This finding opens up new opportunities for aerosol focusing, which is in stark contrast to the classical aerodynamic focusing methodologies. The lines deposited by this method are shown to exhibit widths of 5 micrometers – superior to ink-jet.

Cold Spray Direct-Write. The basic principle of the cold spray process is the following. A high velocity gas jet is used to accelerate solid particles and spray them onto a substrate. The kinetic energy of the particles helps these particles to deform plastically on impact and form splats, which bond together to produce coatings. The speed of solid particles in cold spray process is much higher than speeds of aerosol particles in aerosol beam deposition process. Cold spray is a relatively young process and still considerable efforts are needed to understand and control the process, as well as develop methods to focus the beam of solid particles in a similar way it is done for aerosol beam direct-write.

In the paper mathematical models, numerical algorithms, experimental studies and practical applications of Aerosol Beam and Cold Spray Direct-Write processes will be presented.

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Buchstaber Victor

Corresponding Member of Russian Academy of Sciences

Principal Researcher

Fullerenes and graphene from the point of view of classical and modern mathematics

SCIENTIFIC ORGANIZATION

Steklov Mathematical Institute of RAS

ABSTRACT

The talk is devoted to classical and recent mathematical results, which had drawn attention of physicists and chemists in connection with problems of nanotechnology. R.F.Kurl, H.Kroto, R.E.Smalley were awarded the 1996 Nobel Prize in Chemistry “for their discovery of fullerenes”. A.K.Geim and K.S.Novoselov were awarded the 2010 Nobel Prize in Physics “for groundbreaking experiments regarding the two-dimensional material graphene”. We will discuss combinatorial, geometrical and topological results concerning fullerenes and graphene structures.

KEYWORDS

Molecular carbon structures, convex polytopes, polygonal partitions of 2-surfaces, 4-color problem, 6-manifolds.

Dyachenko Alexander

Doctor of Science

Senior Researcher

Super compact spatial and temporal equations for water waves

SCIENTIFIC ORGANIZATION

Landau Institute for Theoretical physics, Novosibirsk State University

ABSTRACT

We derive very simple super compact equations for unidirectional gravity water waves. Zakharov equation was essentially simplified by some canonical transformation. We suggest a specific form of such transformation that allows one to derive a remarkably simple form of temporal and spatial equatios. One can name it the super compact equation. This equation is very straightforward and includes a nonlinear wave term and advection term. Moreover, this equation also allows one to derive a spatial version of the water waves equation which can be used to describe experiments it the flume.

KEYWORDS

Surface waves, freak waves, hamiltonian approach, numerical simulation.

ACKNOWLEDGEMENTS

This work was supported by Grant “Wave turbulence: theory, numerical simulation, experiment” \#14-22-00174 of Russian Science Foundation.

SUMMARY

We derive very simple compact equations for unidirectional gravity water waves. For such waves, as it is well-known, the coefficient of nontrivial four-wave interaction is identically zero. This fact allows one to essentially simplify the Zakharov equation, applying a canonical transformation. Obviously this transformation is not unique. In this paper we suggest a specific form of such transformation that allows one to derive a remarkably simple form of the Zakharov equation. One can name it the super compact equation. This equation is very straightforward and includes a nonlinear wave term (\`{a} la NLSE) and advection term. Moreover, this equation also allows one to derive a

spatial version of the water waves equation which can be used to describe experiments it the flume.

Efimov Alexander
Scientific Researcher

Non-commutative Jacobian conjecture via triangulated categories

SCIENTIFIC ORGANIZATION

National Research University Higher School of Economics

ABSTRACT

The Jacobian conjecture states that any polynomial self-map of a complex affine space with constant nonzero Jacobian is an isomorphism. I will recall the non-commutative version of this conjecture and explain how it can be proved via triangulated categories.

KEYWORDS

Triangulated categories, localization, representation spaces.

SUMMARY

The main idea is to deduce the non-commutative Jacobian conjecture to a certain statement about localization of triangulated categories.

Faranosov Georgy
PhD
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Aeroacoustics

SCIENTIFIC ORGANIZATION

Central Aerohydrodynamic Institute

ABSTRACT

Azimuthal Decomposition Technique (ADT) allowing extraction subtle features of noise sources of different types is generalized for the case of azimuthally nonuniform microphones distribution with the view of its application to the analysis of large-scale jet noise. It is shown that jet noise measurements by only 3 microphones in each cross-section allow reconstruction of 3 azimuthal modes directivities for low and moderate frequency bands, while 2-microphone measurements make it possible to reconstruct axisymmetric mode directivity and sum directivity of 1st and 2nd modes.

KEYWORDS

Azimuthal decomposition, jet noise.

ACKNOWLEDGEMENTS

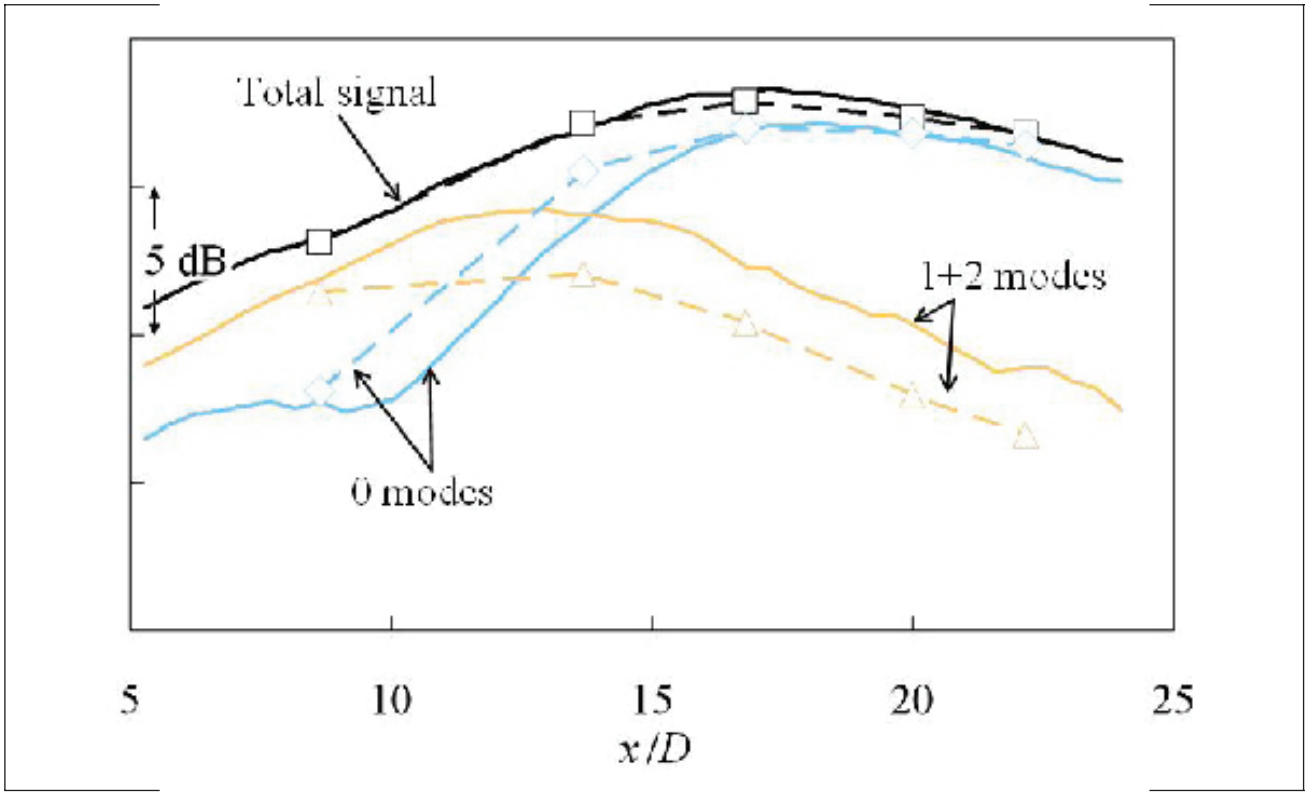
The work was supported by the Russian government under the Government Decree #220: Contract number 14.Z50.31.0032.

SUMMARY

Understanding of the physics of jet noise generation mechanisms is necessary for effective development of noise reduction concepts. Azimuthal decomposition of far-field jet noise, at small-scale models, made it possible to gain insight into the nature of the structure of jet noise sources. In TsAGI, Azimuthal Decomposition Technique (ADT) is realized in anechoic chamber conditions as a standard in-house tool for the investigation of aeroacoustic noise sources. By means of ADT, it was shown that only 3 low-order azimuthal modes contribute to the far-field noise for low and medium frequencies (including spectral maximum), each mode possessing individual, and very nontrivial, directivity. All features of azimuthal modes of jet noise (modal directivities, spectra, cross-correlations) were modeled in our previous works with encouraging accuracy by a special version of correlation approach model based on quadrupole-type sources, for jet velocities from 120 m/s up to 240 m/s. For higher jet velocities, small-scale quadrupoles seems to underpredict jet noise levels, pointing out that another mechanism starts to play a role. One

of the candidates for this mechanism is the noise radiation by instability waves evolving in the jet shear layer. Instability wave concept of jet noise was successfully validated for supersonic jet also on basis of ADT data analysis. Thus, application of ADT to small-scale jets demonstrated its ability to deliver rich information for understanding of noise source features, and its application to full-scale jets of real turbofans is of high interest - it was one of the main task for the Laboratory of Noise Generation Mechanisms and Modal Analisys under the Government Decree #220 (Contract No.14.Z50.31.0032). But implementation of ADT at open test rig faces several challenges: non-free field conditions (due to the presence of the ground) and large geometric dimensions.

In the present work, the results of application of this method to the analysis of large-scale jet noise are presented. It is shown that jet noise measurements by only 3 microphones in each cross-section allow reconstruction of 3 azimuthal modes directivities (axisymmetric, 1st and 2nd) for low and moderate frequency bands, while 2-microphone measurements make it possible to reconstruct axisymmetric mode directivity and sum directivity of 1st and 2nd modes, the microphones being properly located. The latter method is shown to be suitable for utilizing on an outdoor test bench. At first stage, the modified methodology is validated on the small-scale laboratory database, and then it is applied to the jet issuing from the real engine in the ground tests.



Comparison between the results for model scale and large scale jet showed qualitatively similar azimuthal content of the two. Normalized directivity patterns for large-scale and small-scale jets are shown to be in good qualitative conformity in terms of variation of total signal power with Strouhal number, increasing contribution of the axisymmetric mode for downstream observation angles, increasing contribution of 1^{st} and 2^{nd} modes for sideline direction (see figure, where solid lined correspond to the small-sacle jet, and dashed lines - to the full-scale jet). The observed discrepancies may be related to differences in jets structure and operating conditions, simplified data reduction procedure, measurement errors for large-scale-tests or other factors. It is also shown how the proposed method can be extended to allow approximate identification of all 3 azimuthal modes at open test rig.

The results obtained may help in the analysis of the physics of jet noise generation mechanisms for real turbofan engines.

Gilmanova Galia
Master's degree
Researcher

Boundary element simulations of acoustic self-organization in bubbly liquids

SCIENTIFIC ORGANIZATION

Bashkir State University

ABSTRACT

The BEM code was developed and example simulations of formation and propagation of the waves of the acoustically induced transparency in three dimensions were carried out. The results were compared with results obtained earlier other methods and a satisfactory agreement was found.

KEYWORDS

3D Helmholtz equation, boundary element method, bubble dynamics, acoustics of bubbly liquids.

ACKNOWLEDGEMENTS

This study is supported in part by Grant of Ministry of Education and Science of the Russian Federation (11.G34.31.0040), Skoltech Partnership Program.

SUMMARY

Self-organization of bubbles in acoustic fields, or self-action of the acoustic waves in bubbly liquids is a strongly nonlinear phenomenon due to two-way interaction of the bubbles and the acoustic field. A mathematical model of the phenomenon and preliminary computations predict the existence of the waves of self-induced acoustic transparency, which is also confirmed experimentally [1]. Three dimensional particle-in-cell (PIC) simulations tracking all bubbles in the system were performed by the authors earlier [2], where also a good agreement of the theory and experiment was found [1-2].

The PIC simulations however have some deficiency related to the averaging procedure, when the number of particles in the cell is small enough. Such a procedure is required to match the continuum and discrete models of the bubbly liquid each time step. Moreover, in the current version of the PIC code [2] a finite-difference (FD) solver for the Helmholtz equation is used which performance should be improved. In the present study these two problems were addressed by 1) solving the multiple scattering problem for N bubbles (in the limit of a point monopole acoustic source), so there is no need in the continuum model and spatial averaging, and 2) using the boundary element method (BEM) as an alternative to the FD solver. The BEM is modified to include not only boundaries of the domain into the formulation, but also N sources arbitrarily distributed in the computational domain, so both problems are solved at a given time step by a single method. Solution of the problem enables computation of acoustic radiation (Bjerknes) forces on each bubble and, therefore, simulation of the dynamics of the N-body system. Another advantage of the BEM is it capability to solve the problem in domains of complex shape, which has a practical value for design of experimental setups and more realistic simulations.

In the present study a pilot version of the BEM code was developed and example simulations of formation and propagation of the waves of the acoustically induced transparency in three dimensions were carried out. The results were compared with results of [2] and a satisfactory agreement was found. Implementation of the fast multipole method (FMM) for acceleration of the BEM (see [3]) is considered as a future work, which should enable the present method for computations of large systems evolving millions of bubbles.

This study is supported in part by Grant of Ministry of Education and Science of the Russian Federation (11.G34.31.0040), Skoltech Partnership Program

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ADDITIONAL INFORMATION

Galia I. Gilmanova, Nail A. Gumerov, Iskander S. Akhatov.

Glushkov Evgeny
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Piezo-fiber-optic technologies of structural health monitoring for the control of material property degradation, flaw detection and catastrophic failure prevention of aerospace and other safety critical facilities

SCIENTIFIC ORGANIZATION

Kuban State University

ABSTRACT

The project aims to develop Structural Health Monitoring (SHM) technologies for early detection of damages, hidden flaws and material degradation using ultrasonic guided Lamb waves excited and registered by an embedded network of piezoelectric active wafer sensors and/or fiber optic sensors to ensure structural safety of such safety-critical engineering constructions as aircrafts and space units, chemical and nuclear storages, bridges, pipelines, industrial installations, etc.

KEYWORDS

Piezoelectric wafer active sensors (PWAS), fiber Bragg grating sensors (FBG), composite materials, computer simulation, structural health monitoring, damage detection, control of material properties.

SUMMARY

The project aims to create a multidisciplinary laboratory “Piezo-fiber-optic technologies of Structural Health Monitoring” on the basis of the Institute of Mathematics, Mechanics and Informatics (IMMI) and the Laboratory of Robotics and Mechatronics (LRM), KubSU, and to develop Structural Health Monitoring (SHM) methods and technologies for early detection of damages, hidden flaws and material degradation in thin-walled structures using ultrasonic guided waves (Lamb waves) excited and registered by an embedded network of piezoelectric active wafer sensors (PWAS) and fiber optic sensors (fiber Bragg gratings – FBG) or automated (robotic) systems of contactless highly sensitive piezoelectric transducers. Locating, identification and assessment of potential danger of the detected defects are based on a fast mathematical processing of the recorded signals. For its carrying out, it is planned to develop effective computer models that implement semi-analytical and numerical solutions of the corresponding boundary value problems adequately describing wave processes, including in advanced composite materials of complex structure.

The overall objective of SHM technologies is to ensure structural safety of safety-critical engineering constructions, which failure or sudden destruction could lead to serious economic losses or even disastrous consequences. Examples of such objects are aircrafts and space units, chemical and nuclear storages, pipelines, industrial installation, bridges, etc.

The general task of the project is the development of theoretical and technological basics for nondestructive SHM techniques relying on elastic guided waves. Among such expected outcomes as publications in recognized peer-reviewed journals, patents and certificates for computer codes developed, experimental demonstrators and SHM-system prototypes are to be created to illustrate the achievement of the following goals:

1. The assessment of the structural material mechanical properties of modern laminate composites and continuous control of their possible degradation during the structure’s operation via the analysis of signals carried by guided waves.

2. Detection of various hidden flaws typical for plate-like engineering structures (fatigue cracks, delamination of composite interlayers, corrosion of metallic parts and localized material degradation of laminate composites unavailable for visual and classical NDT inspection, impact damages, etc.).

3. Quantification (sizing and estimation of severity) and classification of damages on the basis of wave field pattern acquired by the embedded sensor network and the pattern of scattering resonance frequencies extracted from the registered reflected signals.

4. Continuous structural health monitoring on the basis of built-in piezo/fiber optic sensor networks; self-diagnosis of such built-in systems; assessment of possible further trouble-free operation periods.

As a result of the project, it is planned

- to create the laboratory “Piezo-fiber-optic technologies of Structural Health Monitoring” equipped with modern equipment necessary for carrying out R & D at a world level;

- to prepare from the young project participants (graduate and post-graduate students, postdocs), the backbone of the laboratory, which own the mathematical, computer and experimental methods needed to develop new and improve existing SHM technologies;

- to develop methods and algorithms for the obtaining semi-analytic and numerical solutions of various wave dynamic problems, which effective solving will accelerate the further development of SHM technologies, especially for the structures made of composite materials;- to implement the developed methods in the form of computer models and conduct their experimental verification;

- to create, on this basis, demonstrators, layouts and prototypes of actual SHM systems;

- to apply for patents and certificates for the created objects of intellectual property: computer programs implementing the developed mathematical models and useful models of software and hardware methods.

It is expected that the new scientific and technological products developed during the project will allow early detecting defects, damages and signs of structural aging, thus preventing economic losses and possible catastrophic consequences of their sudden failure or destruction.

ADDITIONAL INFORMATION

The co-author of the presentation is the Leading Scientists of the project Prof. Victor Giurgiutiu, University of South Carolina, USA. He would like to attend the conference and give the lecture personally after the questions of visa and travel support have been resolved.

Grishaev Viktor
PhD in Applied Sciences
Research scientist

Morphology of the impact of particle-laden drops onto solid substrates

SCIENTIFIC ORGANIZATION

Skolkovo Institute of Science and Technology

ABSTRACT

Understanding the impact of particle-laden drops onto substrates is important for many applications, e.g. for additive manufacturing. In our work, the drop impact was studied for dispersions of water and spherical hydrophobic particles with diameters of 200 and 500 μm. The impact was studied by side and bottom view images in the range 150 ≤ We ≤ 750 and 7100 ≤ Re ≤16400 onto hydrophilic (glass) and hydrophobic (polycarbonate) substrates. The particles suppressed the appearance of singular jetting and drop partial rebound but promoted splashing, receding breakup, and rupture.

KEYWORDS
Drop impact, complex drops, particles, wettability.

SUMMARY

The impact of particle-laden drops on substrates is relevant to many technologies, for example, to additive manufacturing, spraying of liquid friction modifiers, etc. These technologies can benefit from a better understanding of the influence of particles on drop impact phenomena.

To understand the influence of the particles, the impact was studied for millimeter droplets. Such droplets are mainly used in impact studies, so they are useful for comparative analysis. As carrier fluid, water was selected. The surface tension of water allows using substrates with different wettability, thereby allowing to cover a maximum number of possible phenomena seen for drop impact on substrates.

The impact velocity was chosen in the range from 1.7 to 3.7 m/s (150≤We≤750 and 7100≤Re≤16400). This allowed us to examine the effect of the particles on various possible number of phenomena (e.g. splashing, deposition, partial rebound, and jetting) occurring during drop impacts with hydrophilic (glass) and hydrophobic (polycarbonate) substrates (Fig. 1).

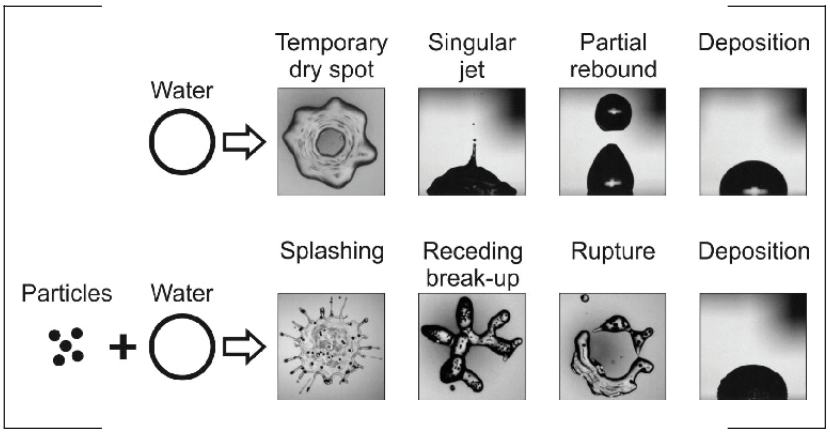

Figure 1. Outcomes of the drop impact onto substrates for water without and with solid particles.

The influence of particles on drop impact phenomena was studied in the case of round iso-dense microparticles with diameter of 200 and 500 μm. The particle diameters were chosen so that they lay in a range in which there are published data to allow comparison. Also, the selected particle sizes are easily distinguishable by high speed video recording systems with a wide field of view (~30x30 mm), which are used in impact studies of millimetric drops. The microparticles were hydrophobic to study the influence of their wettability on comparison with published data obtained for hydrophilic particles.

The addition of 200 μm and 500 μm particles to water drop changed its impact behavior on hydrophilic and hydrophobic substrates (Fig. 1). It was found that the particles suppressed the appearance of singular jetting and drop partial rebound on hydrophobic substrates. Also, on hydrophilic substrates the particles caused early splashing and on hydrophobic substrates the particles caused early splashing, receding breakup and rupture. The occurrences of these phenomena depended on the impact velocity, the particle diameter, and the volume fraction. The increase in drop impact velocity led to an increase in the probabilities for splashing and receding breakup. The increase in particle size caused the increase in the probabilities for splashing, receding breakup and reduction of the probability for partial rebound. The increase in particle volume fraction increased the likelihood of splashing and decreased the likelihood of partial rebound. So, the increase in mentioned parameters decreases the probability of drop deposition without its fragmentation.

The particles changed the spreading dynamics as well. The addition of the 200 μm particles to a water drop led to the fact that its spreading on a hydrophilic substrates happened in two phases: fast and slow. The fast spreading was caused by the action of inertial forces and the slow spreading was caused by the capillary forces, that is, surface wicking. The maximum spreading factor, caused by inertia, reduced linearly with the increase in particle concentration on hydrophilic and hydrophobic substrates. The explanation of this reduction was argued to be the result of energy dissipation through frictional losses between particles and the substrate.

ADDITIONAL INFORMATION

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Graph Surfaces in Non-Holonomic Geometry

SCIENTIFIC ORGANIZATION

Sobolev Institute of Mathematics

ABSTRACT

We investigate graph mappings on non-holonomic structres, deduce their differential properties and prove area formulas.

KEYWORDS

Sub-Lorentzian structure, sub-Riemannian structure, polynomial sub-Riemannian differentiability, area formula.

ACKNOWLEDGEMENTS

The research was supported by Government of Russian Federation (Grant 14.V25.31.0029), RFBR (Grants 14-01-31063-mol-a and 16-01-60036) and Presidium os RAS (Grant 0314-2015-0011).

SUMMARY

Five-dimensional sub-Riemannian and sub-Lorentzian structures are our main topic of research. We consider classes of graph mappings and corresponding graph surfaces on them. It is easy to see that these mappings are not Lipschitz and sub-Riemannian sense and therefore the non-holonomic differentiability theory founded by S. Vodopyanov is not applicable. Nevertheless, our new approach enables us to approximate graph mappings by some polynomials; in other words, they possess the property of *polynomial sub-Riemannian differentiability*, where the “differential” depends polynomially on coordinates of one point with respect to another. The first result is

Theorem 1. *Graph mappings constructed by classes of intrinsically Lipschitz mappings are polynomially sub-Riemannian differentiable.*

The next result is the area formula for corresponding graph surfaces. Emphasize that it depends on values of sub-Riemannian differential of the initial mapping (but not the polynomial differential).

Theorem 2. *If* φ *is a Lipschitz mapping of two one-dimensional Heisenberg groups* $\mathbb{H}$ *and* $\widetilde{\mathbb{H}}$, $\varphi_\Gamma : x \mapsto \exp\left(\sum_{j=1}^{3} \varphi_j(x) X_j\right)(x)$ *is a graph mapping, then the intrinsic sub-Riemanian measure of* $\varphi_\Gamma(\mathbb{H})$ *equals*

$$\int_\Omega \sqrt{1+(X_1\varphi_4)^2(x)+(X_2\varphi_4)^2(x)}\sqrt{1+(X_3\varphi_5)^2(x)}\, d\mathcal{H}^4(x).$$

The intrinsic sub-Lorentzian measure equals

$$\int_\Omega \sqrt{1-(X_1\varphi_4)^2(v)}\sqrt{1-(X_2\varphi_4)^2(v)}\sqrt{1-(X_3\varphi_5)^2(v)}\, d\mathcal{H}^4(v).$$

Here the sub-Lorentzian measure in the image is constructed with respect to “distance”

$$\left(\tilde{d}_\infty^{SL_2}\right)^2(v,y) = \max\left\{\max\left\{y_1^2, y_2^2\right\} - y_4^2, sgn\left(y_3^2 - y_5^2\right)\sqrt{\left|y_3^2 - y_5^2\right|}\right\}.$$

Recently, it also turned out that results similar to Theorems 1 and 2 hold for large classes of graph mappings of Carnot groups, and general area formulas are valid for the corresponding graph surfaces.

Main part of these results are pblished in [1-3].

[1] Karmanova M. B. Area Formula for Graph Surfaces on Five-Dimensional Sub-Lorentzian Structures // Doklady Mathematics, 2016. V. 93, No. 2.

[2] Karmanova M. B. Variations of Non-Holonomic-Valued Mappings and Their Applications to Maximal Surface Theory // Doklady Mathematics, 2016. V. 93, No. 3.

[3] Karmanova M. B. Codimension Two Graph Surfaces over Three-Dimensional Carnot-Caratheodory Spaces // Dokl. AN, 2016. V. 468, No. 6.

Kasimov Aslan

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Quantum dynamics of bouncing droplets

SCIENTIFIC ORGANIZATION

King Abdullah University of Science and Technology

ABSTRACT

This talk is about the dynamics of a fluid droplet bouncing on the surface of a vertically vibrating fluid bath. It was recently discovered that such a droplet can walk along the fluid surface riding a wave created as the droplet hits the surface. In a remarkable series of experiments, this coupled motion of a bouncing droplet and its pilot wave was demonstrated to exhibit a range of quantum effects: discrete orbits, tunneling, single/double slit diffraction, level splitting, scattering, bound states, and others. I will give an overview of these phenomena and discuss their implications.

KEYWORDS

Fluid mechanics, bouncing droplets, quantum effects.

SUMMARY

For some further details, see:

http://web.kaust.edu.sa/faculty/aslankasimov/research-experiments.shtml

Kopiev Victor

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Development of innovative methods of investigation of noise generation mechanisms by turbulent flows

SCIENTIFIC ORGANIZATION

Central Aerohydrodynamics Institute (TsAGI) and Perm National Research Polytechnic University (PNRPU)

ABSTRACT

The main results are: (i) Creation of the new anechoic facility which enables turbulent jet and vortex ring noise investigation; (ii) Development of azimuthal decomposition technique (ADT) for measurements by means of reduced number of microphones adapted to open rig; (iii) application of noise source localization technique (beamforming) to real aircraft engine; (iv) Development of methods for measurement and analysis of sound field modal structure in the engine inlet; (v) Development of liner impedance eduction methods for the engine ducts and methods of liner manufacturing.

KEYWORDS

Aeroacoustics, jet noise, vortex rings, microphone array, source localization, jet and inlet azimuthal modes, liner impedance eduction.

Kraiko Alexander
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A new model of the big bang and the universe expansion. A comparison with modern observational data and cosmological theories

SCIENTIFIC ORGANIZATION

Baranov Central Institute of Aviation Motor Development

ABSTRACT

The new model of the Big Bang and Universe expansion is constructed. It is based on so-lutions in classical and in relativistic statements of problem on dispersion in void of the gas compressed “in a point” or “almost in a point” (further - “problems on dispersion”).

KEYWORDS

Big Bang, Universe expansion, dispersion in a void

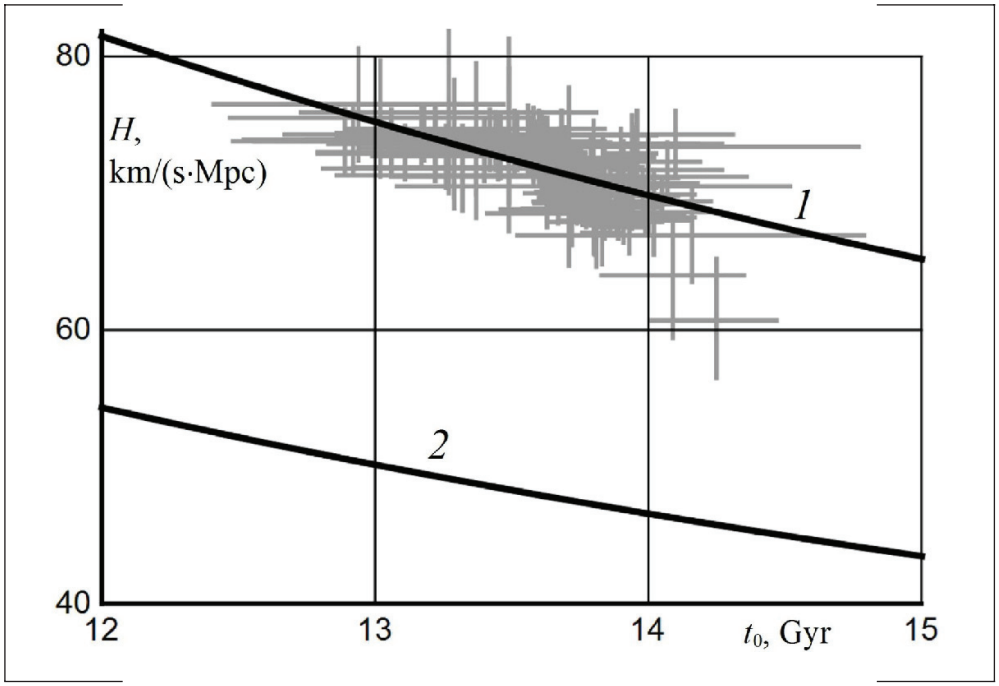
ACKNOWLEDGEMENTS

The investigation is carried out at support of RFBR (projects 14-01-00146 and 14-01-31057).

SUMMARY

A. Einstein, trying to describe the stationary Universe within the general theory of relativity (GRT), has introduced in GRT a constant Λ, called “a cosmological constant”. Regardless to the Universe A. Friedman has constructed in 1922 the non-stationary solution within GRT with $\Lambda = 0$. Scalar parameters of the medium and certain “a scale factor” in this solution are functions only of time, and speed **u** in co-moving coordinates is zero. In 1929 E. Hubble, measuring Doppler shift of light of the remote galaxies, has formulated the law according to which far galaxies move away from us with speed of **u** proportional to radius vector **r** to them: **u** = *H*(*t*)**r**. Time-dependent *t* function *H*(*t*) is called “Hubble’s constant”. If galaxies scatter, then if we have the suitable solution, it is possible to define, when they were together, i.e. when they (more exactly, gas particles from which galaxies were created then) “have scattered from a point or almost from a point”. Friedman solution has been taken as suitable after Hubble discovery. In it the singularity moment, when the density is infinite everywhere, is taken for the always boundless Universe expansion beginning, and the scale factor is equal to zero. Time t_0, which is read from this moment, is the Universe “life” time. Possibility of Universe expansion description with A. Friedman’s solution did not cause doubts till 1998, when two groups of American astronomers have discovwered its discrepancy to observational data. For elimination of the discovered discrepancy A. Friedman’s solution has been generalized on nonzero Λ, which choice has allowed to conform observations with this solution. Like A. Einstein approach, the computed values of Λ lead to effect of antigravitation. Three representatives of the mentioned groups have received Nobel Prize in 2011 for such antigravitation discovery and accompanying it accelerated Universe expansion. Unknown for the present carrier of anti-gravitation, connected with Λ, is called “dark energy”.

In 2015 authors of the report have solved in classical and in relativistic statements a problem on dispersion in a void of the gas compressed in a point or in its small vicinity (further - “a problem on dispersion”) [1]. Comparisons of the simple solution obtained (in both statements speed of u = r/t, i.e. H (t) = 1/t) with the same observational data surprisingly have shown, that it without attraction of any empirical constants describes the data not worse than any modern cosmological theory (ΛCDM) with dark energy (Λ) and matter (CDM - Cold Dark Matter). In the solution obtained (at $t = +0$ and $0 \le r/(ct) \le 1$, *c* is the speed of light) the pressure *p*, the specific (units of volume) enthalpy *w* and the internal energy e = *w* – *p* instantly vanish, i.e. e instantly transforms to the kinetic energy of the gas. Validity of the told confirms figure with more than two hundreds NASA variants of four most reliable observational data sets processing with tens modern cosmological theories [2] which form area, covered with grey crosses (vertical and horizontal parts of crosses give errors of Hubble constant *H* definition and the Universe lifetime t_0). A curve *1*, defined by a formula $H = 978/t_0$ which is the sequence of the solution **u** = **r**/*t*, passes through the area, here *H* in km / (s×Mpc), t_0 in Gyrs.



Grey crosses are the reliable observational data processed with modern

cosmological theories (%5CLambda%20CDM) [2]; curve 1 corresponds to the formula $H = 978/t_0$,

curve 2 – to the formula $H = 652/t_0$,which is a consequence of Friedman solution with $\Lambda = 0$

The formula **u** = **r**/*t* at the description of the extending Universe is used throughout almost all E. Milne's monograph [3]. Milne has obtained it, however, not from the solution of a problem on dispersion of the gas compressed in a point, but on the basis of cosmological principle formulated $\Lambda = 0$ by him and additional, sometimes not enough reasonable assumptions. Milne finishes with a formula **u** = (2/3)**r**/*t*, which is a consequence of Friedman solution with $\Lambda = 0$ for Universe expansion from thermodynamically nonrelativistic gas. For the reasons specified, after Milne the formula **u** = **r**/*t*, entered by him, was not involved in the description of the Universe expansion. In the figure the curve *2* corresponds to the solution **u** = (2/3)**r**/*t*, which is lying much lower than covered with crosses area.

Due to the dark energy which has appeared with introduction %5CLambda%20%5Cneq%200, we read [4]: "The discovery of dark energy dotted the i's and crossed the t's in observational cosmology. The standard cosmological model (%5CLambda%20CDM) fitting the whole set of observational data arose for the first time in the development of science. Nowadays, it has no serious rivals". Comparison of the covered with crosses area in the figure with the curve 1 testifies to appearance of such competitor without any uniform empirical constant, without dark energy and a matter. If the dark matter can be necessary for the description of Universe expansion slowdown, in the light of the solution constructed above, there is no need of dark energy.

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Mechanical properties of amorphous and crystalline TiNiCu thin ribbons

SCIENTIFIC ORGANIZATION

Saint-Petersburg State University

ABSTRACT

This work is dedicated to the investigation of mechanical properties of TiNiCu-alloy. Samples were obtained from a thin melt-spun amorphous ribbon. The first objective was to examine dependance of mechanical properties of amorphous specimens on the experiment temperature. The second objective was to obtain crystallized samples and study their mechanical behaviour depening on annealing regimes, so a few temperatures above the temperature of crystallization to prepare crystallized specimens were chosen.

KEYWORDS

Amorphous alloys, melt-spun ribbons, shape memory alloys, thermal processing, mechanical behavior.

ACKNOWLEDGEMENTS

Grant of the Government of the Russian Federation designed to provide governmental support to scientific research projects implemented under the supervision of the world's leading scientists at Russian institutuions of higher learning, research institutions subordinare to the RF Federal Agency for Scientific Organizations and governmental scientific research centers of the Russian Federation № 14.B25.31.0017 of 28 June 2013.

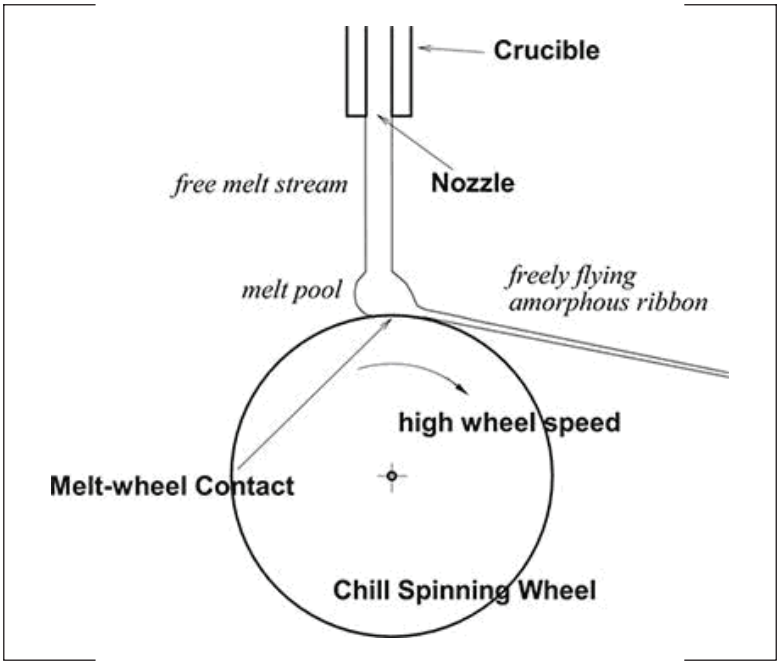
SUMMARY

Introduction

Nowadays shape memory alloys become very popular among scientists and manufacturers due to their remarkable properties. And titanium nickelide (TiNi) is one of the best known representatives of such alloys.

There is a possibility to obtain some TiNi-alloys with initially amorphous state using melt-spun technique. It is known that mechanical behaviour of amorphous materials is strongly dependent on the temperature, so it is very important to investigate properties of amorphous TiNiCu melt-spun ribbons at different temperatures.

To make amorphous ribbons capable of undergoing martensite transformations it is necessary to crystallize them. This could be carried out by heating the material above the temperature of crystallization. Besides, alloy microstructure and mechanical properties could vary considerably depending on the heating temperature, annealing duration and other crystallization parameters. So this dependance is a subject of a second part of the work.



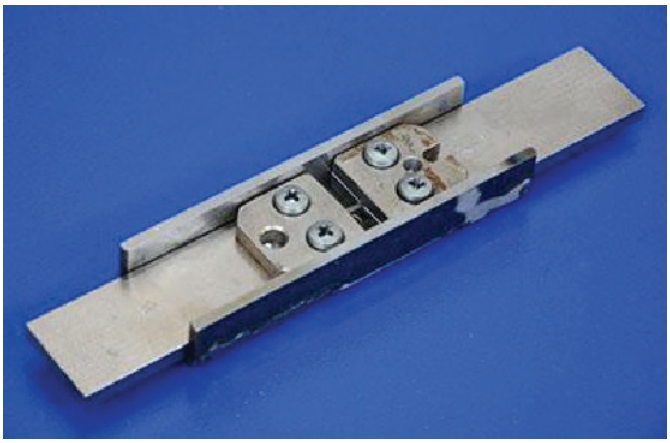
Objects and methods

Samples made from thin Ti50Ni50Cu25 amorphous ribbons of 1.6 mm in width and 35 μm in thickness were inversigated.

Three-component alloy was chosen for survey because of the requirement of cooling with critical cooling rate or higher, and this rate decrease with the increasing of alloy components quantity.

The research of mechanical behaviour was conducted using tensile machine Shimadzu AG-XD plus while the temperature was mantained in the heat-chamber Shimadzu TCE-N300.

Specimens were set in specially designed and produced grips which were fixed in machine holders.



The tape was cut into pieces of 35 mm in length. Value of the gauge length turned out to be about 8 mm accoding to standards so then the appropriate grips were made.

Some specimens in the amorphous state were subjected to tension process at different temperatures. Another set of experiments was carried out on samples subjected to annealing in a furnace to become crystallized. Heating was conducted at 5°C/min from room temperature up to temperatures of 470, 500, 550, 600 and 650°C - temperatures above the crystallization temperature. Whereafter the final temperature was maintained during one hour.

RESULTS

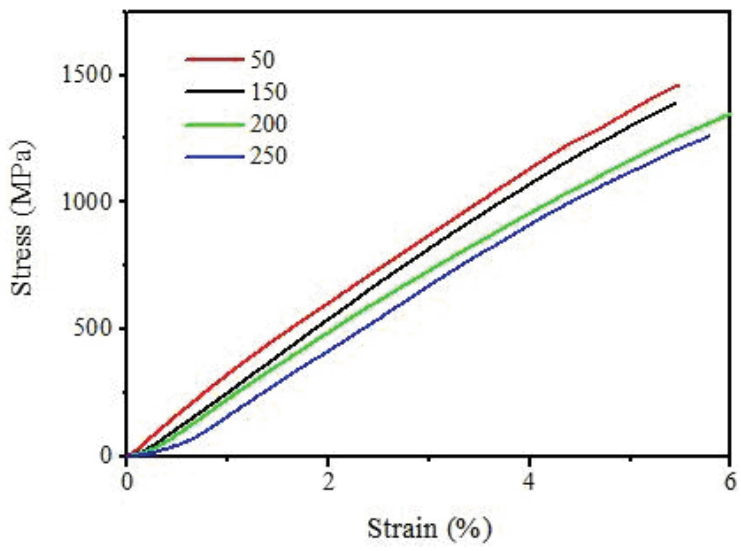


Fig. 1. Stress-strain diagram of amorphous specimens at different temperatures.

Table 1

Young's modulus of amorphous specimens at different temperatures

Temperature, °C	50	150	200	250
Young's modulus, 102 MPa	318	280	266	257

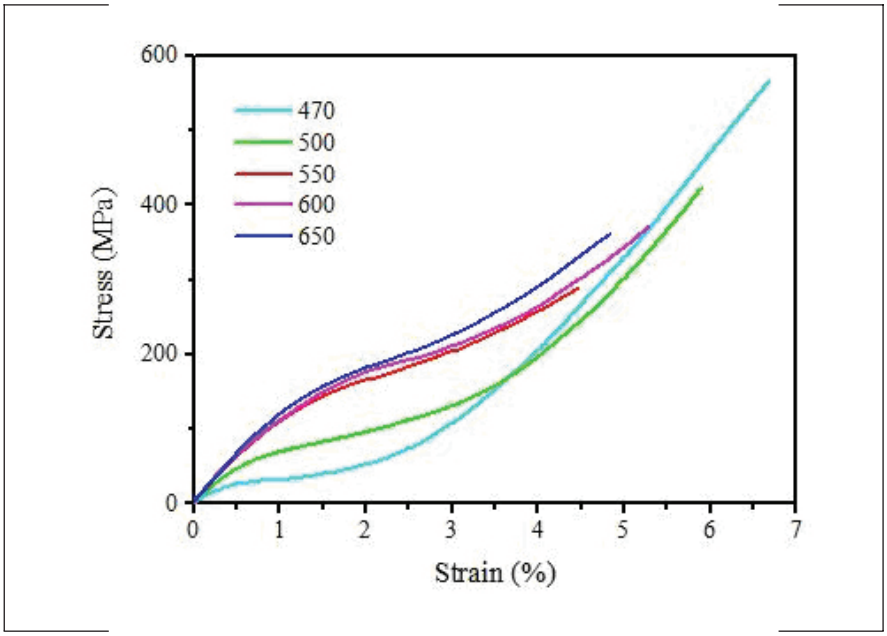


Fig. 2. Stress-strain diagram of crystallized specimens annealed at different temperatures and deformed at 20°C.

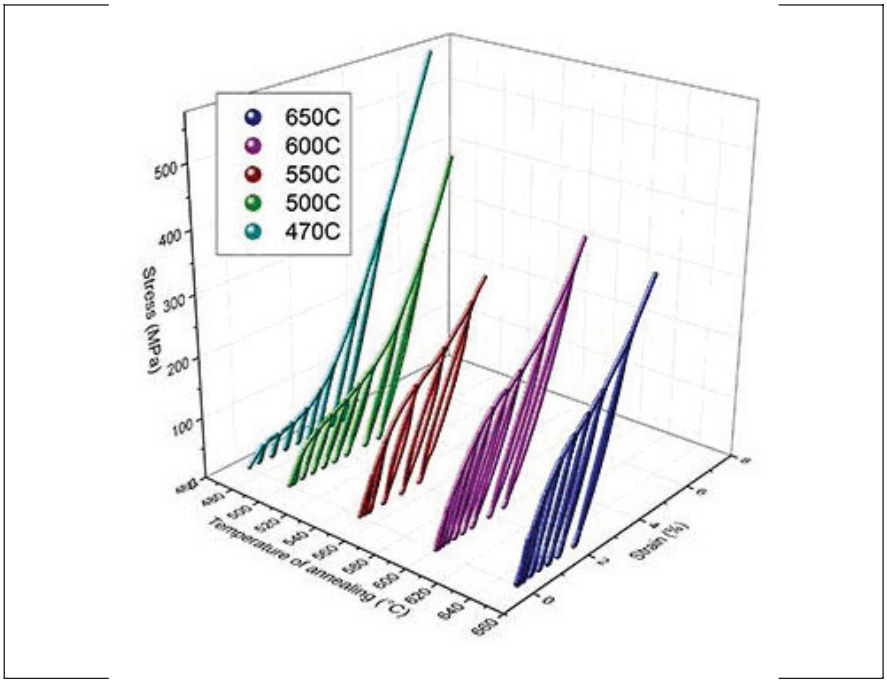


Fig. 3. 3D-diagram of crystallized specimens annealed at different temperatures and deformed at 20°C.

Table 2

Stress corresponding to the start of inelastic deformation due to the martensite reorientation (martensite reorientation limit) for crystallized specimens annealed at different temperatures and deformed at 20°C.

Temperature of annealing, °C	470	500	550	600	650
Martensite reorientation limit, MPa	20	49	123	132	129

Table 3

Inelastic deformation accumulated due to the martensite reorientation at full strain of 5% for crystallized specimens annealed at different temperatures and deformed at 20°C.

Temperature of annealing, °C	470	500	550	600	650
Inelastic deformation, %	3,3	3,2	---	2,5	---

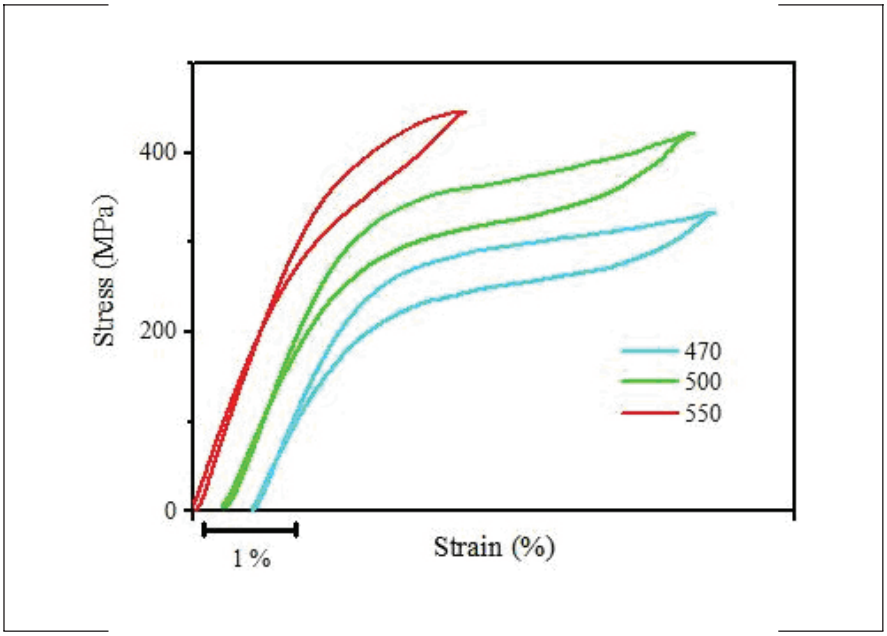


Fig. 4. Stress-strain diagram of crystallized specimens annealed at different temperatures and deformed at 20°C.

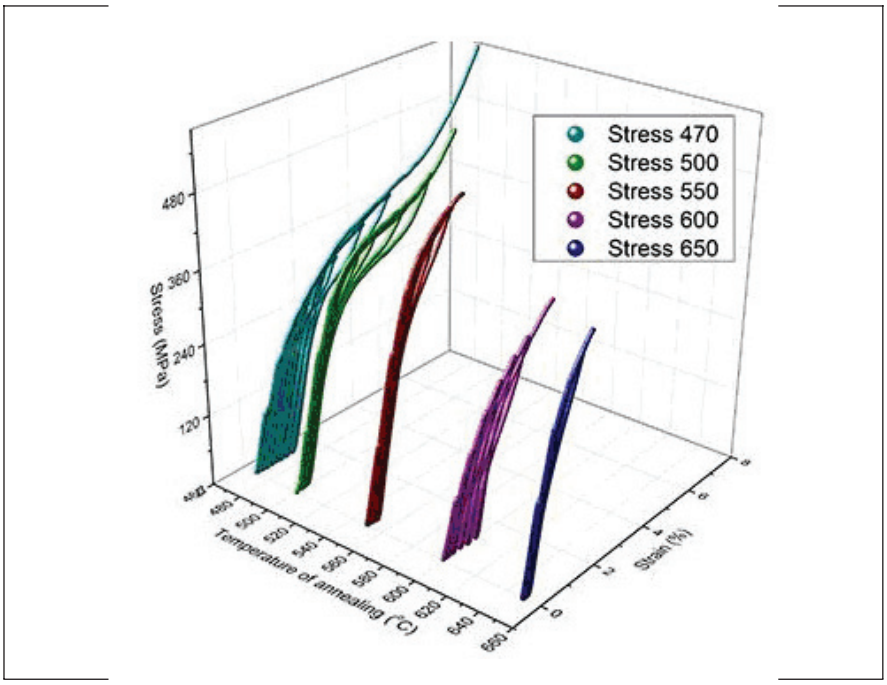


Fig. 5. 3D-diagram of crystallized specimens annealed at different temperatures and deformed at 90°C.

Table 4

Young's modulus of austenite phase for crystallized specimens annealed at different temperatures and deformed at 90°C.

Temperature of annealing, °C	470	500	550	600	650
Young's modulus, 102 MPa	262	294	319	343	315

Table 5

Phase yield stress values for crystallized specimens annealed at different temperatures and deformed at 90°C.

Temperature of annealing, °C	470	500	550	600	650
Phase yield stress, MPa	240	303	356	281	282

Conclusions

- Amorphous melt-spun $Ti_{50}Ni_{25}Cu_{25}$ ribbons deform elastically until fracture within a temperature range of 20-250°C. Young's modulus decreases with the increasing of deformation temperature.
- Crystallized melt-spun $Ti_{50}Ni_{25}Cu_{25}$ ribbons which were subjected to annealing at different temperatures demostrate pseudoelastic behaviour at austenite phase. Phase yield stress depends on annealing temperature.
- Crystallized melt-spun $Ti_{50}Ni_{25}Cu_{25}$ ribbons deform inelastically due to the mechanism of martensite reorientation at martensite phase. Stress corresponding to the start of inelastic deformation and value of the accumulated inelastic deformation depend on annealing temperature.

Plans for further investigations

It would be interesting to use Digital image correlation optical method for local strain measurement in future. This method allows to obtain pictures with strain fields of the whole specimen during the test so it helps in finding shear bands and initial destruction point.

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Three-dimensional wave regimes on vertically falling liquid films: Downstream evolution of statistical characteristics

SCIENTIFIC ORGANIZATION

Novosibirsk State University

ABSTRACT

The experimental study of 3D wave characteristics as well as study of transition process from 2D to 3D waves for liquid films falling down a vertical plate was conducted. The LIF method was used to obtain instant shapes of waves. During 2D-3D wave transition, a strong transverse redistribution of liquid leading to the formation of rivulets on the surface of liquid film takes place. Obtained data were used to calculate various statistical characteristics such as dispersion, PDF and PSD.

KEYWORDS

Laser induced fluorescence, 3D wavy liquid film, PDF, PSD.

ACKNOWLEDGEMENTS

Russian Science Foundation Grant No. 14-22- 00174.

SUMMARY

Three-dimensional (3D) wave regimes are considered to be the last stage of the film flow evolution at moderate Reynolds numbers. In such regimes surface of the film is covered with numerous 3D waves. Therefore statistical approaches are often involved in order to describe these wave regimes.

Results of experimental study of 3D wave characteristics as well as study of transition process from two-dimensional (2D) to 3D waves for liquid films falling down a vertical plate are presented. Experiments were carried out in the range of Reynolds numbers 5 < Re < 100.

Liquids with various physical properties were used as working fluids. The whole flow structure was registered using shadowgraph method. It was found that rivulets formation takes place during the process of transition from 2D to 3D wave motion. Size of the forming rivulets is weakly affected by Re, however rivulets' evolution depends on flow parameters. Detailed structures of the waves were studied by means of the high speed laser induced fluorescence (LIF) method, which makes it possible to obtain instantaneous forms of 3D waves. Obtained film thickness data were used to calculate various statistical characteristics such as dispersion values, probability density functions (PDF), spectral power densities of film thickness fluctuations, mean film thickness distribution etc. Extensive statistical analysis showed that rivulets' behavior is depending on prior characteristics of 2D waves in the upper part of film flow. Immovable or randomly shifting in transverse direction rivulets can be observed. On time-averaged (t=0.7s) cross sections different amount of rivulets can be observed for different moments in time. The statistical analysis also allows us to suggest that stabilization of 3D wave motion occurs at relatively short distances from liquid inflow for the flow regimes with high Reynolds numbers whereas at lower Re continuous downstream evolution of the wave characteristics with gradual damping of the waves is observed.

Musin Airat

PhD

Senior Researcher

Experimental and mathematical modeling of fluid flow in microchannels with varying void volume in relation to the question of studying the fluid flow in hydrocarbon source rocks

SCIENTIFIC ORGANIZATION

Bashkir State University

ABSTRACT

In work the method of experimental study is developed for dynamics of changes of filtration and capacitance parameters of void space. Numerical simulation is made for physical experiment contained in simulation of active fluid flow through the channel fabricated in polymer and followed by swelling and deswelling of polymer. A number of physical parameters are empirically estimated. A qualitative agreement is obtained for simulation and experimental results. For the first time ever in the work the using of polymer swelling is introduced for imitation of kerogen.

KEYWORDS

Filtration, microchannel, soft litography, polymer swelling, mathematical modeling.

ACKNOWLEDGEMENTS

This study is supported in part by Grant of Ministry of Education and Science of the Russian Federation (11.G34.31.0040), Skoltech Partnership Program.

SUMMARY

A shale plays mining is followed with changes of filtration and capacitance parameters due to physical and chemical transformations of kerogen during a filtration in oil source rocks. Complex kinetics of such processes should be considered in mathematic simulation that is required a development of new experimental methods for their verification.

In work the method of experimental study is developed for dynamics of changes of filtration and capacitance parameters of void space. Experimental setup is made

for recording of flow parameters in microchannels corresponding to physical model of filtration medium by way of polymer microfluidic device made by using soft lithography. Dynamic change of microchannel permeability is reached by virtue of polymer swelling when interacting with active fluids (alkanes, esters).

Dynamic parameters of fluids flow in fabricated microchannels are obtained (water, alkanes, esters). It's found that used active liquids lead to essential change of microchannel permeability under their flow through the microchannel.

Mathematical model is developed for the flow of active fluid through the channel with permeability changed dynamically due phenomena described above.

Numerical simulation is made for physical experiment contained in simulation of active fluid flow through the channel fabricated in polymer and followed by swelling and deswelling of polymer. A number of physical parameters are empirically estimated. A qualitative agreement is obtained for simulation and experimental results.

For the first time ever in the work the using of polymer swelling is introduced for imitation of kerogen releasing from oil source rock that leads to change of filtration parameters. The procedure is developed for physical and numerical experiments for determination of filtration and capacitance parameters of the model during of active agent flow in microchannels with permeability changed dynamically.

ADDITIONAL INFORMATION

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Symmetry properties of dynamics of two-phase medium

SCIENTIFIC ORGANIZATION

Chelyabinsk State University

ABSTRACT

There is considered a system of partial differential equations, which describes dynamics of two-phase medium. Algebra Lie of symmetry group of this system is found. Invariant and partially invariant solutions are found by using symmetry group. Some of solutions describes mixing phases in one- and three-dimensional space.

KEYWORDS

Two-phase medium, invariant solutions, symmetry group, partially invariant submodels, Lie algebra.

ACKNOWLEDGEMENTS

The author expressses gratitude to the Laboratory of Quantum Topology and Chelyabinsk State University for a support by grants under which some of this work was carried out.

SUMMARY

There is considered a system of partial differential equations, which describes dynamics of interpenetrating movement of two compressible mediums. This system is investigated using methods of group analysis: symmetry groups, invariant solutions, optimal system of subalgebras. Research gave the following results. Algebra Lie of symmetry group is found. Invariant and partially invariant solutions of this system are found. Some of solutions describes mixing phases in one- and three-dimensional space.

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Post graduate student

On Hamiltonian geometry of the associativity equations

SCIENTIFIC ORGANIZATION

Lomonosov Moscow State University

ABSTRACT

In the case of three primary fields, the associativity equations (the WDVV equations of the two-dimensional topological quantum field theory) can be represented as integrable nondiagonalizable systems of hydrodynamic type (O.I. Mokhov). There arose the classification problem of the existence of a local homogeneous first-order Hamiltonian structure of the Dubrovin-Novikov type for systems of hydrodynamic type which are equivalent to the associativity equations. O.I Mokhov and the author have completely solved this problem. These results will be presented.

KEYWORDS

The associativity equations, Hamiltonian structures of the Dubrovin-Novikov type.

ACKNOWLEDGEMENTS

This research was supported by RSF 16-11-10260.

SUMMARY

In the case of three primary fields, the associativity equations (the WDVV equations of the two-dimensional topological quantum field theory) can be represented as integrable nondiagonalizable systems of hydrodynamic type (O.I. Mokhov). The Hamiltonian geometry of these systems depends on the metric of the associativity equations: there are examples, which have local homogeneous first-order Hamiltonian structures of the Dubrovin-Novikov type, and examples, which do not have such structures (O.I. Mokhov and E.V. Ferapontov). So there arose the classification problem of the existence of such a Hamiltonian structure for the associativity equations. O.I Mokhov and the author have completely solved this problem. These results will be presented.

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Mathematical problems of quantum control

SCIENTIFIC ORGANIZATION

National University of Science and Technology «MISIS», Steklov Mathematical Institute of RAS

ABSTRACT

Quantum control studies possibilities to manipulate atomic and molecular systems with quantum dynamics using an external field, e.g., a shaped laser pulse. It is an important area of research which attracts high interest due to existing and prospective applications in quantum technologies ranging from quantum information and computing to laser control of chemical reaction and photochemistry. In this talk we will discuss various mathematical topics in quantum control and outline resent results in this field.

KEYWORDS

Quantum control, quantum technology, quantum information.

SUMMARY

Quantum control studied possibilities to manipulate atomic and molecular systems with quantum dynamics using an external control field, e.g., a shaped laser pulse. It is an important area of research which attracts high interest due to various existing and prospective applications in quantum technologies ranging from quantum information and computing to laser control of chemical reaction and photochemistry.

Examples of applications include breaking a chemical bond by laser, manipulation by a qubit, etc. In each quantum control problem the goal is to find a shape of the control pulse which optimally achieves the control goal. The control goal can be mathematically represented as a functional of the control pulse. The control problem can be formulated as maximization of the objective functional. In this talk we will outline some problems in quantum control including analysis of complete controllability of open quantum systems and investigation of quantum control landscape which is the graph of the objective functional. Specific property of the quantum control landscape is the number of traps, i.e. local but not global optima. This property has pratical importance as determining the level of difficulty of finding globally optimal controls. Recent results in this field include proof of the absence of traps for state manipulatin and gate generation for a single qubit, absence of traps for control of quantum transmission, the existence of trapping behaviour for multilevel quantum systems with special symmetries, etc.

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SCIENTIFIC ORGANIZATION
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Boundary element simulations of 3D bubble-droplet-particle dynamics

ABSTRACT

To simulate dynamics of large bubble/droplet/particle systems the boundary element method accelerated both via the fast multipole method, and heterogeneous computing architecture is developed. Three-dimensional emulsion flows in channels, dynamics of deformable bubble or droplet, bubble self-propulsion, interaction between bubbles and rigid particles or solid wall in the presence of external forces are presented.

KEYWORDS

Multiphase flow, bubble, droplet, particle, microchannel, boundary element method, fast multipole method, graphics processors.

ACKNOWLEDGEMENTS

This study is supported in part by Grant of Ministry of Education and Science of the Russian Federation (11.G34.31.0040), Skoltech Partnership Program, RFBR grant 16-31-00029, Christian Doppler Research Association (Austria), Goettingen University (Germany), and Fantalgo, LLC (Maryland, USA).

SUMMARY

Investigation of complex multiphase flows consisting of gas, liquid, and solid phases is of significant interest for science and many new technologies. This includes various biomedical applications, microfluidics, environmental and manufacturing technologies. The boundary element method (BEM) is a suitable tool for modeling of the dynamics of large bubble/droplet/particle systems at low and high Reynolds numbers (Stokesian and potential flows). Application of the conventional BEM for the direct simulation of such systems is normally limited by the memory, computational complexity, and speed. To achieve such simulations a numerical approach based on the BEM accelerated both via the fast multipole method (FMM), and heterogeneous computing architecture (multicore CPUs and graphics processors) is developed. The method enabled direct simulations of systems of tens of thousands of deformable dispersed objects in an unbounded domain or near a solid wall.

We focused on the simulation of three-dimensional emulsion flows in channels of arbitrary cross-section, dynamics of exited high order surface modes of bubbles at free and forced bubble oscillations, bubble self-propulsion, transfer of energy between shape and volume modes of bubble oscillations, interaction between bubbles and rigid particles or solid wall in the presence of external forces. Several demonstration computations for the dilute emulsions in microchannels and surface attached bubble are compared with experimental data.

The developed approach can be used for solution of a wide range of problems related to disperse flow in microscale. As a future work we also consider extension of the physical model and appropriate algorithmic modifications which take into account effects of the close object interaction.

This study is supported in part by Grant of Ministry of Education and Science of the Russian Federation (11.G34.31.0040), Skoltech Partnership Program, RFBR grant 16-31-00029, Christian Doppler Research Association (Austria), Goettingen University (Germany), and Fantalgo, LLC (Maryland, USA).

ADDITIONAL INFORMATION

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Experimental study of dynamics of viscous bubbly liquids in ultrasound

SCIENTIFIC ORGANIZATION

Bashkir State University

ABSTRACT

Experiments with viscous bubbly liquids exposed to mild acoustic fields ~ 100 kHz demonstrate a propagating of bubbles from a sound source and leaving almost clear liquid behind it. It's found three typical shapes of bubble front that depend of intensity of acoustic field.

KEYWORDS

Acoustics, experiments, dynamics, bubbly glycerol, ultrasound.

ACKNOWLEDGEMENTS

This research was supported by the Grant of the Ministry of Education and Science of the Russian Federation (11.G34.31.0040) and Skoltech Partnership Program.

SUMMARY

Self-organization of bubbles in acoustic field is a strong nonlinear effect owing to two-way field-bubbles interaction. Oscillating pressure gradient and bubbles volume give rise to averaged Bjerknes force which involves bubbles drift much slower than period of the acoustic field. As bubbles disperse and dissipate the sound, their movements lead to changes of the field. In turn this leads to manifestation of interesting nonlinear effects such as self-induced transparency [1] and filamentous structures formation [2, 3]. Experiments showed the formation of volume fraction with high bubbles concentration on a bubble front propagating from sound source and leaving almost clear liquid behind it [4].

One of important parameters controlling the process is a viscosity of liquid. Study of its influence on a velocity of the transparency wave propagation is especially important during a liquidation of microbubbles occurring during a degassing of very viscous liquids in petroleum and glass industry, for example.

In this research there are experimental results of studies which are a continuance of previous work [4]. In the present study, the processes of viscous bubbly liquids cleaning by acoustic field are much slower, time intervals are more than 10^4 longer. So for present experiments a current experimental setup is modified through a fabricating of an additional cooling chamber to avoid of PZT overheating. The high-speed camera is turned into a low-speed one by adding of a signal generator to it allowing the camera to take pictures with another frequency range (0.5 – 2 frames per minute). Bubbles of two different gases (air and helium) are generated in the liquid by using the Venturi tube. As viscous medium an aqueous solution of glycerol of different viscosity is used.

Exposing the bubbly glycerol by ultrasound it is found that it leads to bubbles propagating from sound source and leaving almost clear liquid behind it. It's also

found three typical shapes of bubble front that depend of intensity of acoustic field.

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ADDITIONAL INFORMATION

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Dimensionless analysis of self-ignition of hydrocarbons during the high-pressure air injection process based on numerical simulation

SCIENTIFIC ORGANIZATION

Bashkir State University

ABSTRACT

In this work we consider a one-dimensional mathematical model of the self-ignition and propagation of combustion zone in conditions of a non-isothermal three-phase filtration with phase transitions and chemical reactions in the undeformable porous media. In the process of analysis of the mathematical model the original dimensionless complexes were selected. On the basis of performed computations the diagnostic graph, that allows to determine the possibility of application of the in-situ combustion technique, is constructed.

KEYWORDS

Self-ignition, in-situ combustion, mathematical modeling, dimensionless analysis.

ACKNOWLEDGEMENTS

This study is supported in part by Grant of Ministry of Education and Science of the Russian Federation (11.G34.31.0040), Skoltech Partnership Program, RFBR grant 16-31-00423.

SUMMARY

Air injection into the reservoir accompanied by in-situ combustion is a complex process in which heat and mass transfer phenomena, heat conduction, heat transfer, phase transformations and chemical reactions take place. Interaction between these processes is characterized by a set of dimensionless parameters. In this work we consider a one-dimensional mathematical model of the self-ignition and propagation of combustion zone in conditions of a non-isothermal three-phase filtration with phase transitions and chemical reactions in the undeformable porous media. Mathematical model includes equations for mass balance of phases and components, and equations for energy balance, supplemented by the corresponding closing relations. The following assumptions are used: liquid phases are considered to be in-compressible; the gas phase is compressible and defined by the ideal gas law; the gas consists of water vapor, oxygen and inert gas; gas components are insoluble in oil and water; heat exchange with the surrounding rocks is considered. The system of equations of mathematical model is solved numerically with the usage of finite volume method and IMPES-method. In the process of analysis of the mathematical model the original dimensionless complexes were selected. These complexes are composed by parameters of Frank-Kamenetskii, Peclet, Bio and oil saturation, which characterize interactions of the aforementioned processes during

the in-situ combustion. The results of multi-parametric analysis of the in-situ combustion problem based on these dimensionless complexes are presented. On the basis of performed computations the diagnostic graph, that allows to determine the possibility of application of the in-situ combustion technique, is constructed.

ADDITIONAL INFORMATION

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Experimental analysis of effects of core joints on axial fatigue of composite sandwich structures

SCIENTIFIC ORGANIZATION

Skolkovo Institute of Science and Technology

ABSTRACT

In practice, sandwich core sheets are joined with a simple butt-joint before infusion. The intensity of the axial load transferred thru core-to-core joint might influence the performance of the sandwich structure. This research work tends to examine this effect under static and fatigue loading. Finite element analysis was used to validate the specimens' geometrical configurations. Experimental results for butt-, finger- and scarf-type joints are presented and discussed.

KEYWORDS

PVC, foam, fatigue, core, S-N curve, scarf, junction.

ACKNOWLEDGEMENTS

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SUMMARY

Results obtained are summarized in the following:

- Results from axial static tensile test did not reveal any significant difference in strength among all joint configurations.
- In comparison with the traditional butt joint, the scarf joint increased the axial stiffness of the sandwich panel by 16 %.
- The fatigued specimens featuring the scarf joint outperformed the traditional butt joint and the baseline design (without core joint). Fatigue life with respect to facing stress increased by 6 %.
- The proposed core finger joint showed a shallower trend line (S-N curve) than the butt and scarf joints, indicating higher relative fatigue performance at high-cycle levels.

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Composite materials adhesion and cohesion properties research

SCIENTIFIC ORGANIZATION

Oryol State University

ABSTRACT

The main property is the strength of the composite. It is caused by adhesion of its elements. It is proposed to solve the problem of selection of the elemental composition based on the idea of nonlocal potential many-particle interactions of its infinitesimal elements. Characteristically, the parameters of the potentials of interparticle interactions approximating functions are defined on the basis of the classical experiments to determine the characteristics of the linear elastic state of the composite elements.

KEYWORDS

Mechanics of solids, solid state physics.

SUMMARY

1 Introduction

While consider adhesion of solid bodies based on non-traditional models of local Cosserat, Leroux, Tupin, Mindlin, Aero for the calculation of mechanical processes with specific constructional elastic materials, the problem of determining the elastic constants arise. The methods of solid-state physics for such materials are difficult or impossible to use. The mechanical processes in such materials are described on the basis of the phenomenological approach conveniently. This approach is based on the continuum thermodynamics. Therefore, methods for calculating the characteristics of the elastic state mediums with internal degrees of freedom should be based on the phenomenological of the macro experiment.

One of the phenomenon, whish described by the models of Cosserat, Leroux, Tupin, Mindlin, Aero, is the adhesion. The characteristics of adhesion are its energy and adhesive force. In this paper, the elastic constants are determined by calculation. It is based on the nonlocal elastic medium.

2 Theoretical positions

The interaction of bodies $B \equiv B_{(k)}$ ($k = 1,2,...$ – number of body) is considered. These bodies are bounded by smooth surfaces $A \equiv A_{(k)}$. Surfaces have the outward unit normal $\vec{n} \equiv \vec{n}_{(k)}$. The bodies $B \equiv B_{(k)}$ composed of homogeneous, isotropic linear elastic materials. Each of them is considered dedicated from the infinite medium $\Omega \equiv \Omega_{(k)}$. The material $\Omega \equiv \Omega_{(k)}$ and $B \equiv B_{(k)}$ is the same. This assumption excludes the influence of the material properties of the body $B \equiv B_{(k)}$ by its boundary region. The state $B \equiv B_{(k)}$ inside $\Omega \equiv \Omega_{(k)}$ is the reference. It corresponds to time $t = 0$.

Every body $B \equiv B_{(k)}$ can be presented as a union of non-intersecting parts $\Delta B_n \equiv \Delta B_{(k)n}$. The density of materials $\rho \equiv \rho_{(k)}$ and their temperatures $T \equiv T_{(k)}$ are distributed uniformly and do not change over time. Thus: $T_{(1)} = T_{(2)}$.

The particles – material points.

In the reference configuration arbitrary body *B* occupies the region *V* and center of inertia of its particles have a *dB* radius vectors $\vec{r} \in V$. The position of an arbitrary particle dB_2 relative to other arbitrary particle $dB_1 \equiv dB$ is defined relative radius vector $\vec{l}_{12} = \vec{r}_2 - \vec{r}_1$ with length $l_{12} = |\vec{l}_{12}| = |\vec{r}_2 - \vec{r}_1|$.

Under the influence of external mechanical impacts, including the allocation of $B \equiv B_{(k)}$ from $\Omega \equiv \Omega_{(k)}$, particles $dB \equiv dB_{(k)}$ acquire new provisions, which are characterized by the radius vectors $\vec{R} \equiv \vec{R}_{(k)} \in V_{t(k)}$ and the displacement vector $\vec{u}(\vec{r},t) = \vec{R}(\vec{r},t) - \vec{r}$. Area $V_{t(k)}$ – is the area, which occupied by the body $B \equiv B_{(k)}$ in the current configuration. The position of a particle

dB_2 relative particle $dB_1 \equiv dB$ will change and will be determined by the radius vector $\overrightarrow{L_{12}} = \overrightarrow{R_2} - \overrightarrow{R_1} = (\overrightarrow{r_2} - \overrightarrow{r_1}) + (\overrightarrow{u_2} - \overrightarrow{u_1}) = \overrightarrow{l_{12}} + \Delta\overrightarrow{u_{12}}$ and length $L_{12} = |\overrightarrow{L_{12}}| = |\overrightarrow{R_2} - \overrightarrow{R_1}|$. If $B \equiv B_{(k)}$ body is deformed, then $L_{12} \neq l_{12}$.

It is assumed that the deformations are small: $|L - l|/l << 1|$. Therefore, the density of the material equality and volumes of elementary particles in the reference and current status are equal.

Vectors $\Delta\overrightarrow{u_{1,j}}$ can be represented as a series in exterior powers $\overrightarrow{l_{1,j}}$.

$$\underbrace{}_{n\ times} \qquad\qquad \underbrace{}_{n\ times}$$

$$\Delta\overrightarrow{u_{1,j}} = \sum_{n=1}^{\infty} \frac{1}{n!} \left(\nabla_{1,j}^n \vec{u}\right) \cdot \ldots \cdot \overrightarrow{l_{1,j}^n} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \left(\nabla^n \vec{u}\right) \cdot \ldots \cdot \left(\overrightarrow{l_{1,j}}\right)^n, \quad j = 2,3,\cdots, \qquad (1)$$

where $\nabla = d\ldots/d\vec{r}$ – differential del operator on a vector $\overrightarrow{r}$, and $\nabla_{1,j} = d\ldots/d\overrightarrow{l_{1,j}}$ – on a vector $\overrightarrow{l_{1,j}}$.

It is believed that the vector $\overrightarrow{r_{(1)}}$ receives the increment $d\overrightarrow{r_{(1)}}$, then the vector $\overrightarrow{l_{1,j}}$ receives the increment $d\overrightarrow{l_{1,j}} = -d\vec{r}$. It means: $\nabla_{1,j}^n = (-1)^n \nabla^n$.

The distortion tensor is the gradient of the curvature tensor. It is expressed by the second gradient of the displacement vector.

$$\nabla\nabla\vec{u} = \nabla^2\vec{u} = u_{i,jn}\vec{e_i}\vec{e_j}\vec{e_n} = D_{ijn}\vec{e_i}\vec{e_j}\vec{e_n} = d_{ij,n}\vec{e_i}\vec{e_j}\vec{e_n} \qquad (2)$$

If the characteristics of the kinematics of the continuum is necessary to use a second gradient of displacement, then it may appear dislocation.

In known scientific works is formulated kinematic sign of adhesion of the two bodies. Any material fiber, which intersects the contact surface $A_{(12)}$, should preserve the smoothness of the distribution of their deformation. It is suggested that this characteristic may be made by using the curvature tensor for a description deformations (2). This means that for the adhesion of elastic materials must arise field dislocations. When there is adhesion of two metals, this feature is enough.

If there is metal adhesion, then allowed, that the total potential energy of the combined body $B = B_{(1)} \cup B_{(2)}$ is the sum of the potential energies of many-particle interactions inside each of the bodies $B_{(1)}$ and $B_{(2)}$, and between them. The quantities, $\Phi_{(kpq)}^{(2)}(\overrightarrow{R_{(k)}}, \overrightarrow{R_{(p)}}, \overrightarrow{R_{(q)}})dV_{(k)}dV_{(p)}dV_{(q)}$, … are the potentials of pair, triple, etc. interactions of particles pair $dB_{(k)}, dB_{(p)}, dB_{(q)}$ bodies $B_{(k)}, B_{(p)}, B_{(q)}$ $k,p,q = 1,2$. In this case, $dV_{(k)}, dV_{(p)}, dV_{(q)}$ – the volume of the interacting particles in the reference state. Functions (the potential) $\Phi_{(kp)}^{(2)}(\overrightarrow{R_{(k)}}, \overrightarrow{R_{(p)}}), \Phi_{(kpq)}^{(2)}(\overrightarrow{R_{(k)}}, \overrightarrow{R_{(p)}}, \overrightarrow{R_{(q)}})$ for a homogeneous isotropic material depend only on the distance between the interacting particles in the current state.

The energy $dW_{(1)}(\overrightarrow{R_{(1)}}) = w_{(1)}(\overrightarrow{R_{(1)}})dV_{(1)}$ of infinitesimal particle, e.g., $dB_{(1)}$ with the volume $dV_{(1)}$ and center of inertia $\overrightarrow{R_{(1)}}$ is presented in the form of

$$w_{(1)}(\overrightarrow{R_{(1)}})dV_{(1)} = (w_{(11)} + w_{(12)})dV_{(1)} =$$
$$= \left[\Phi_{(11)}^{(2)}dV_{(1)} + \tfrac{1}{2!}\int_{V_{(1)}}\int_{V_{(1)}} \Phi_{(111)}^{(3)}dV_{(1)}dV_{(1)} +]\ldots\right]dV_{(1)} +$$
$$+ \left[\int_{V_{(2)}} \Phi_{(12)}^{(2)}dV_{(2)} + \tfrac{1}{2!}\sum_{k=1}^{2}\int_{V_{(2)}}\int_{V_{(k)}} \Phi_{(12k)}^{(3)}dV_{(k)} + \ldots\right]dV_{(1)}$$

In this equality $w_{(11)}$ – the cubic density of the potential energy, which arose due to the interaction of the particles of the body $B_{(1)}$ among themselves; $w_{(12)}$ – addition to the quantity of $w_{(11)}$, which arises from the interaction particles of the body $B_{(1)}$ with the particles of the body $B_{(2)}$. Each particle $dB_{(1)} \subset B_{(1)}$ is affected by the forces from the other particles $dB_{(1)}$ of the same body $B_{(1)}$, particles

$dB_{(2)}$ body $B_{(2)}$ and the medium, which surrounds both the body. The first forces are called forces of cohesive interaction parts of the body. Their cubic density is: $\overrightarrow{f_{(11)}} = -\nabla w_{(11)}$.

The second forces are adhesive forces. Their cubic density is:

$$\overrightarrow{f_{(12)}} = -\nabla w_{(12)} = -\overrightarrow{f_{(21)}}. \quad (3)$$

During the deformation of the material interacting particles $dB_{1(k)}$ and $dB_{j(p)}$ experienced relative displacements $\Delta\overrightarrow{u_{1j}}$. For the particles decomposition (1) is valid. At the same time, pair, triple, etc. potential interaction is permissible to submit second-order polynomials relatively $\Delta\overrightarrow{u_{1j}}$. Absolute term of the polynomial and its coefficients are expressed in the potentials of many-particle interactions in the reference state.

Changing the cubic density $\Delta w_{(11)}$of the potential energy body $B_{(1)}$ is a function of the sequence $\{\nabla^n \overrightarrow{u}\}$ displacement gradients. If we differentiate dependence $\Delta w_{(11)}(\nabla\overrightarrow{u}, \nabla^2\overrightarrow{u}, \ldots)$ by the gradients $\nabla^n\overrightarrow{u}$, we obtain the expression for the stress tensor, which develop in the material body $B_{(1)}$.

$$P^{(n)} = \frac{\partial \Delta w_{(11)}}{\partial(\nabla^n \vec{u})} = P^{0(n)} + \sum_{m=1}^{\infty} \underbrace{(\nabla^m \vec{u})\cdot\ldots\cdot}_{m\ times} C^{(m,n)}, \quad (4)$$

where $P^{0(n)}$ – tensor of initial stress; $C^{(m,n)}$ – tensors, which characterize the mechanical properties of the material. Taking into account only pair and triple interactions, the defining relations have the form:

$$P^{0(m)} = \frac{1}{2!}\int_V \frac{1}{m!}(\nabla_{12}\Phi^{(2)}_{(11)})\overrightarrow{l^m_{12}}dV_2 + \frac{1}{3!}\sum_{j=2}^{3}\int_V\left[\int_V \frac{1}{m!}(\nabla_{1j}\Phi^{(3)}_{(111)})\overrightarrow{l^m_{1j}}dV_2\right]dV_3, \quad (5)$$

$$C^{(n,m)} = \frac{1}{2!}\int_V \frac{1}{m!n!}\overrightarrow{l^n_{12}}(\nabla_1^2\Phi^{(2)}_{(11)})\overrightarrow{l^m_{12}}dV_2 + \frac{1}{3!}\sum_{p,q=2}^{3}\int_V\left[\int_V \frac{1}{m!n!}\overrightarrow{l^n_{1p}}(\nabla_p\nabla_q\Phi^{(3)}_{(111)})\overrightarrow{l^m_{1q}}dV_2\right]dV_3. \quad (6)$$

Jump to a specific local model is the replacement of (1) the sum of one, two, etc. terms. Herewith, sequence $\{P^{(n)}\}$ stored a corresponding number of cells.

The equation of motion for interacting bodies $B_{(1)}$ and $B_{(2)}$ in stresses for the local model has the form:

$$\rho_{(k)} = \frac{\partial^2\overrightarrow{u_{(k)}}}{\partial t^2} = \nabla\cdot\left(P^{(1)}_{(k)} - \nabla\cdot\left(P^{(2)}_{(k)} - \nabla\cdot\left(P^{(3)}_{(k)} - \ldots\right)\right)\right) + \overrightarrow{f_{(kp)}} + \psi_{(k)}, \quad (7)$$

$$k,p = 1,2;\ k \neq p$$

where $P^{(m)}_{(k)}$, $m = 1,2,3,\ldots$ – internal stress tensor.

The field of vectors $\overrightarrow{\psi_{(k)}} = \overrightarrow{\psi_{(k)}}(\overrightarrow{r_{(k)}})$ are defined. The fields $\overrightarrow{f_{(kp)}} = \overrightarrow{f_{(kp)}}(\overrightarrow{r_{(k)}}, \overrightarrow{r_{(p)}})$ are defined by (3). The value $w_{(12)}$ is calculated through the interaction potentials of particles in the assumption of the absence in these strains. The interaction potentials must be known.

At time $t = t_{0(k)}$ We set the initial conditions of the displacements distribution and velocities of the particles of the body $B_{(k)}$, which occupied an area of $V_{(k)}$.

Therefore, the use of expressions (7) and (4) – (6) makes a conjugate problem of the contact interaction of elastic bodies with regard to their adhesion. In the reference state, the potentials of all the many-particle interactions should be known.

3 The results of calculation

Expressions (5) and (6) show, that the characteristics of the elastic state of the material are calculated by the potentials of nonlocal interaction of its particles. The feature of metals – pressure of the electron gas is taken into account in known

scientific works. Nonlocal interaction potentials-material point are requested to identify with a nonlinear dispersion law. The dispersion law – the dependence of $w^2 = f(K^2)$ is determined experimentally. It is approximated by a polynomial of degree n. The value of the degree n is determined by the condition of current task. Geometrical conditions of adhesion is the continuity and smoothness of field variations for those displacements of contacting bodies, which they obtained by adhesion. For performing the conditions is sufficient to apply only the first two displacement gradients in the description of the deformations, which occur in the adhesion of the two bodies. It's enough to take $n = 2$.

In this case, depending on the potential pair and triple interactions are approximated by functions

$$\Phi^{(2)}_{(kp)} = \Phi^{(2)}_{0(kp)}\left(e^{-2\beta_{(kp)}l_{12(kp)}} - 2e^{-\beta_{(kp)}l_{12(kp)}}\right),$$
$$\Phi^{(3)}_{(k,p,q)} = \Phi^{(3)}_{0(k,p,q)}\left(e^{-2\beta_{(kp)}l_{12(kp)}} - 2e^{-\beta_{(kp)}l_{12(kp)}}\right)\left(e^{-2\beta_{(kq)}l_{13(kq)}} - 2e^{-\beta_{(kq)}l_{13(kq)}}\right). \quad (8)$$

These functions are equal to zero at an infinite distance. These particles may belong to the body $B_{(k)}$ $(k = p = q)$ or another $(k \neq p \vee k \neq q)$.

In the first case $(k = p = q)$, for the parameters $\Phi^{(2)}_{0(kp)}$, $\Phi^{(3)}_{0(kpq)}$, $\beta_{(kp)}$ were obtained calculating formulas.

$$\left(\frac{\Phi^{(2)}_{0(k)}}{\beta^3_{(k)}}\right) = \frac{4\mu_{(k)} + 45\lambda_{(k)}}{294\pi} = \frac{E_{(k)}}{294\pi}\frac{2 + 41\nu_{(k)}}{(1+\nu_{(k)})(1-2\nu_{(k)})} \quad (9)$$

$$\left(\frac{\Phi^{(3)}_{0(k)}}{\beta^6_{(k)}}\right) = \frac{27(\lambda_{(k)} - \mu_{(k)})}{1764\pi} = \frac{27E_{(k)}}{1764\pi}\frac{4\nu_{(k)} - 1}{2(1+\nu_{(k)})(1-2\nu_{(k)})} \quad (10)$$

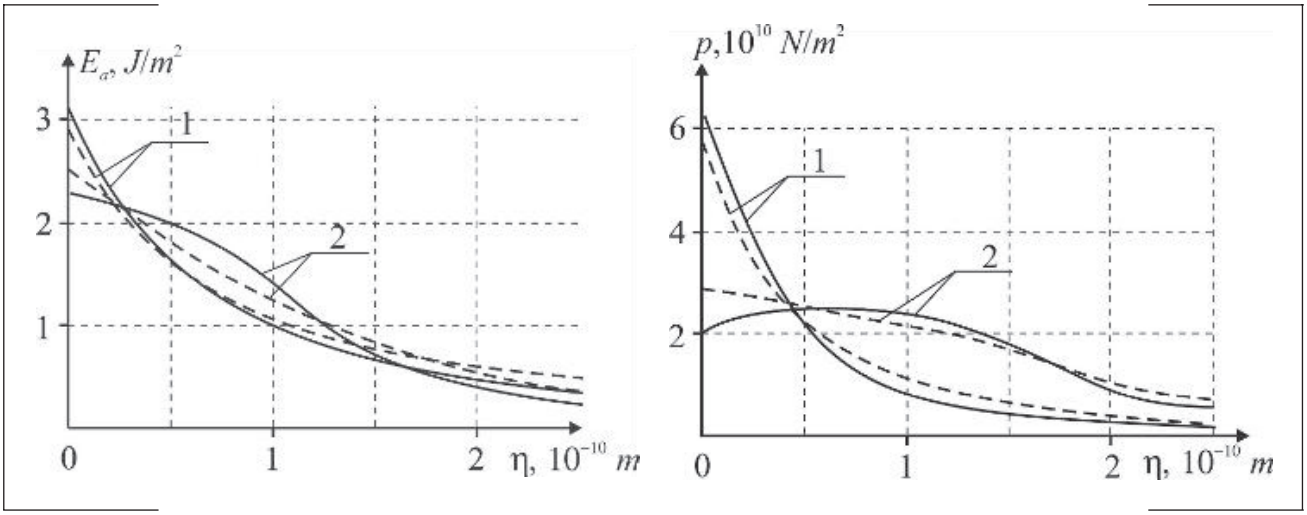
$$\beta_{(kk)} = \frac{1}{2}\sqrt{3\pi\left(\frac{f_{0(kk)}}{f_{1(kk)}}\right)\frac{15\left(\frac{\Phi^{(2)}_{0(kk)}}{\beta^3_{(kk)}}\right) + \left(\frac{1563\pi}{4}\right)\left(\frac{\Phi^{(3)}_{0(kk)}}{\beta^6_{(kk)}}\right)}{2\mu_{(kk)} + \lambda_{(kk)}}} \quad (11)$$

Formulas (9) and (10) are the result of the comparison Voigt notation for tensor traditional characteristics of the elastic state of the material with the first term of the polynomial $w^2 = f(K^2)$. Equations (9) and (10) are constructed with help (5) and (8).

Equation (11) is obtained by comparing the first and second terms the submission of the dispersion law $w^2 = f(K^2)$ for of plane longitudinal waves in the form of a polynomial of the second degree.

In the second case $(k \neq p \vee k \neq q)$, when the bodies of different materials interact, for determining the parameters $\Phi^{(2)}_{0(kp)}$, $\Phi^{(3)}_{0(kpq)}$, $\beta_{(kp)}$ are used depending on the characteristics of elastic state two-component solid solutions from the concentration of their components.

The methodology, which is proposed, allowed to calculate the interaction potential semi-infinite bodies $B_{(1)}$ and $B_{(2)}$ (fig. 1, a), the force of attraction of *p* (fig. 1, b), which depends on the distance between the h units of area boundary planes $A_{(1)}$ and $A_{(2)}$. The results of calculation are compared with existing works. Conformity is satisfactory.



a) b)

Fig. 1. The dependence of the potential E_a and the force of attraction p from the distance η for combinations $Cu-Al$ – curves 1 and $Al-Al$ – curves 2.

Staroverov Oleg
Researcher

Study vitality and behavior of composite materials under the combined shock, cyclic and quasi-static loadings

SCIENTIFIC ORGANIZATION

State National Research Polytechnical University of Perm

ABSTRACT

The study of behavior of composite materials samples under combined loadings and developed and perfected technique of estimation of residual strength (vitality) panel's samples in terms of the contact impact was carried out in Center of Experimental Mechanics. Diagrams of dependence of the residual strength of the glass-carbon fiber sample plates and panels were presented in work. The characteristic features of the behavior of the samples at pre-contact compression and impact loading to failure. For a more detailed analysis of the failure of samples used video system Vic-3D.

KEYWORDS

Composites materials, combined loadings, failure of composites.

ACKNOWLEDGEMENTS

This study was carried out at the Perm National Polytechnic University with supportof the Government of Russian Federation (Decree No. 220, April 9, 2010) under Contract No. 14. B25.310006, June 24, 2013.

SUMMARY

The study of behavior of composite materials samples under combined loadings and developed and perfected technique of estimation of residual strength (vitality) panel's samples in terms of the contact impact was carried out in Center of Experimental Mechanics.

Diagrams of dependence of the residual strength of the glass-carbon fiber sample plates and panels were presented in work. It analyzed the fracture compression. The characteristic features of the behavior of the samples at pre-contact compression and impact loading to failure. For a more detailed analysis of the failure of the samples used in compression-contact optical video system Vic-3D, the mathematical apparatus which is based on the method of digital image correlation.

Studies of the behavior of composites under quasi-static and cyclic combined actions were carried out on samples of woven fiberglass. The obtained experimental

data of residual degradation properties diagrams were constructed according to the number of load cycles prior. Mechanisms of destruction was analyzed.

The paper presents the methodology of composites under impact tests and quasi-static tension, as well as an estimation of change of deformation and strength properties.

The paper suggested further ways of development of techniques associated with the experimental investigation of the behavior of composites under cyclic samples, and the impact of quasi-static loading.

ADDITIONAL INFORMATION

Wildemann V.E., Lobanov D.S., Belonogov N.S., Spaskova E.M.

Stepanov Robert
Master in Science
Junior researcher

Investigation of velocity fields of rotor wake for hover mode

SCIENTIFIC ORGANIZATION

Kazan National Research Technical University named after A.N.Tupolev (KNRTU-KAI)

ABSTRACT

In this work, experimental results for tip vortices, trailing behind rotor blades in hover mode, are presented. The study was conducted on the rotor rig in the T-1K wind tunnel (KNRTU-KAI). The obtained results were used to identify shapes and sizes of the vortices.

KEYWORDS

PIV, vortex core, rotor.

SUMMARY

In this work, experimental study results of velocity field measurements in the vicinity of tip regions of rotor blades are presented for hover mode. The measurements were obtained using stereo PIV Dantec system.

Obtained velocity fields were used to idenify vortex core shapes in the first approximation using four intermediate points. Due to unsymmetrical nature of the vortex cores, their radii were determined from equivalent circles, which had same area as the obtained closed loop of the vortex shape.

Also, the trajectory of the vortices in the rotor wake is presented.

Turov Mikhail
Researcher

Martinet-Ramis modulus for one Quadratic System

SCIENTIFIC ORGANIZATION

Chelyabisk State University

ABSTRACT

For quadratic vector field dp/dv=(p(1-v))/(v(p-v)) was determinate coefficients of the modulus Martinet-Ramis.

KEYWORDS

Martinet-Ramis modulus, saddlenode.

SUMMARY

There are consider a quadratic system $\begin{cases} \dot{p} = p(1-v) \\ \dot{v} = v(p-v) \end{cases}$ (1)

This system is in a some sense, limit system for well known Jouanolou system. The system (1) has a saddlenode singularity at the origin.

In this work we calculate first coefficients of Martinet-Ramis' modulus .

Martinet-Ramis' modulus (C, ϕ) (for saddlenode singular point) are constructed by transformations reducing initial system to its (orbital) formal normal form. Solutions of the system (1) with given initial conditions can be found as a series (with respect to initial condition). Using these solutions it is possible ti find coefficients of the normalizing transformations, and then to determinate coefficients of modulus.

As a result we get

Theorem: Let (C, ϕ) be Martinet-Ramis modulus for (1).

Then: $C = 0, \phi(z) = z + 2\pi i z^2 + (2\pi i - 4\pi^2) z^3 + \ldots$

Corollary: The system (1) is not analytically orbital equivalent to its formal normal form.

Yankin Andrey
Researcher

Mechanical behavior of the viscoelastic polymers under two-frequency loads

SCIENTIFIC ORGANIZATION

State National Research Polytechnical University of Perm

ABSTRACT

In this work, nonlinear representations of stress and strain under two-frequency loadings were presented, and it was proposed to describe dynamic modules and loss angles by polynomials and to use a time-temperature superposition for determining dependencies of the viscoelastic parameters on the temperature; to determine viscoelastic parameters, it was proposed to use the Fourier series.

KEYWORDS

Highly-filled viscoelastic polymer composites (elastomers), two-frequency (dual-frequency) loadings, complex dynamic modulus, loss angle, dynamic mechanical properties (analysis)

ACKNOWLEDGEMENTS

The work was carried out in the Perm National Research Polytechnic University with support of the Government of Russian Federation (The decree № 220 on April 9, 2010) under the Contract № 14.B25.310006, on June 24, 2013.

SUMMARY

The topic relevance is due to: the use of highly-filled polymer composites in important aerospace structures and other industries; the action of complex harmonic loadings on structures where highly-filled polymers are used; the need to develop methods of experimental research and to define deformation properties of materials and calculation methods for structures working in extreme conditions.

The aim of this research is to develop methods for conducting the dynamic experiment, to define viscoelastic parameters of highly-filled polymer composites under stationary two-frequency loadings, and to identify the mathematical model for calculating the stress-strain state of viscoelastic aerospace structures.

As a result of this work, nonlinear representations of stress and strain under two-frequency loadings were presented, and polynomials was used to describe dependencies of dynamic modules and loss angles on frequency. A time-temperature superposition was also used for the accounting of the viscoelastic properties on the temperature, and the Fourier series to determine the viscoelastic parameters.

Future work includes developing optimal experimental design, determining material constants, and checking the model adequacy.

ADDITIONAL INFORMATION

R.V. Bulbovich.

Zamula Yuriy
Higher education
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Studying the mechanical properties of geological rock samples at micro- and nano- scales with atomic force microscopy-based techniques

SCIENTIFIC ORGANIZATION

Bashkir State University

ABSTRACT

The effective elastic modulus of rock samples from a West Siberian unconventional oil field were mapped at micrometer resolution using two AFM nanoindentation techniques: (1) building “force-distance” curves in nanoindentation mode of AFM and (2) operation of AFM probe in oscillating intermittent contact mode. The obtained results were compared to the data acquired with a dedicated nanoindenter device from the same rock samples.

KEYWORDS

Atomic force microscopy, mechanical properties, rocks, elastic modulus.

ACKNOWLEDGEMENTS

This research is supported by the Grants of the Ministry of Education and Science of the Russian Federation (11.G34.31.0040) and Skoltech Partnership Program.

SUMMARY

Studying mechanical properties of rock is an important part of a geomechanical characterization workflow applied to geological formations, containing recoverable hydrocarbon resources, consumable water, or holding CO2 or nuclear waste. Traditional mechanical tests are mostly focused on studying centimeter-sized rock samples with provision of integral mechanical characteristics of rock. Application of Atomic Force Microscopy (AFM) to mechanical studies of geological materials allows resolving integral mechanical characteristics down to properties of individual grains and intergranular interfaces. AFM technology helps to acquire a deep insight into internal structure of rock, to understand rock mechanics at micro-scale, and to forecast rock behavior under different stimulation regimes, with the help of additional numerical modeling.

Geological rock samples are composite materials often consisting of a large number of mineral and organic phases. Due to natural anisotropy of certain rocks, the values of their mechanical properties experience a broad variation within mineral and organic phases. This variation is typically observed at micro- and nano-scale; these effects effects can be successfully captured with an AFM technique. Comprehensive AFM analysis of rock samples includes mapping of effective elastic modulus of mineral and organic phases over the sample area, studying anisotropy of mechanical properties within particular grains and characterization of intergranular interfaces.

In this work, the effective elastic modulus of rock samples from a West Siberian unconventional oil field were mapped at micrometer resolution using two AFM nanoindentation techniques: (1) building “force-distance” curves in nanoindentation mode of AFM and (2) operation of AFM probe in oscillating intermittent contact mode. The obtained results were compared to the data acquired with a dedicated nanoindenter device from the same rock samples.

This research is supported by the Grants of the Ministry of Education and Science of the Russian Federation (11.G34.31.0040) and Skoltech Partnership Program.

ADDITIONAL INFORMATION

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Petr Zhilyaev
PhD
Junior researcher

Molecular dynamics simulation of surface tension

SCIENTIFIC ORGANIZATION

Skolkovo Institute of Science and Technology

ABSTRACT

Interfacial phenomena in thin films, bubble and droplet have great interest for researchers for quite a long time because of wide applications as well as because of their statistical uncertainties in engineering and science realms. Since molecular movements and interactions are critical to estimate the characteristics of the interface, the molecular dynamics (MD) is a good way to approach that problem.

KEYWORDS

Molecular dynamics, surface tension.

SUMMARY

The main goal of this work is to give a systematic estimation of surface tension for planar and spherical cases and related characteristics using the molecular dynamics (MD). For planar case, a thin film is considered. For spherical case, a droplet and a bubble are considered. Distributions of density and pressure tensor components are obtained through an averaging process during MD trajectory. The surface tension for planar case is obtained directly from pressure tensor. Base on the mechanical arguments for the force and moment balances and the mechanical stability called as “mechanical route” bubble and droplet surface tensions are calculated together with the corresponding radii. Also dependence of surface tension on cut-off radius, temperature and size of the system is investigated.

ADDITIONAL INFORMATION

Co-authors: Iskander Akhatov Professor, Director of the Skoltech Center for Design, Manufacturing and Materials.

NEW MATERIALS, MANUFACTURING TECHNOLOGIES & PROCESSES

Bardakova Kseniia
Junior researcher

Chitosan derivatives 3D structuring via laser stereolithography and two-photon polymerization

SCIENTIFIC ORGANIZATION

Crystallography and Photonics RAS

ABSTRACT

Three-dimensional structures was formed on the basis of chitosan derivatives by two-photon polymerization, laser stereolithography and micromolding methods. The optimum ratio of the components, methods of preparation of photopolymerizable mixtures, parameters of the laser structuring, method of removing a non-crosslinked material were suggested. We studied cytotoxicity, proliferative activity, the degree and nature of the activation of expression of differentiation marker genes for stem cells, the compatibility of the primary cells of the nervous system.

KEYWORDS

Two-photon polymerization, micromolding, laser stereolithography, regenerative therapy, matrices, biocompatible materials.

ACKNOWLEDGEMENTS

Laser Zentrum Hannover e.V.: Boris N. Chichkov; Institute of Photonic Technologies, Research center “Crystallography and Photonics”: Victor N. Bagratashvili, Peter S. Timashev, Nikita V. Minaev, Anastasia V. Koroleva.

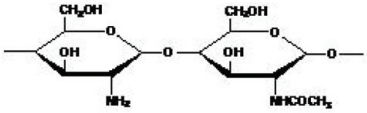
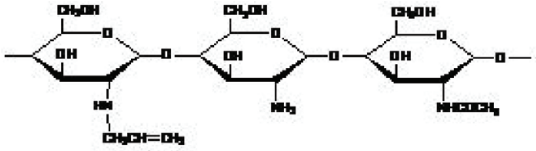
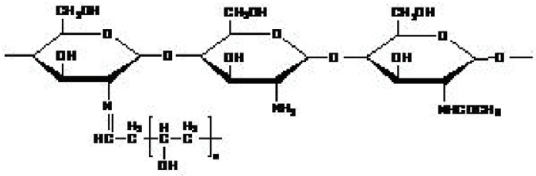
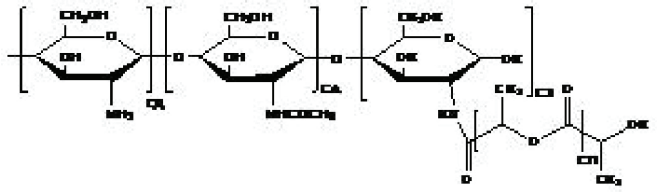
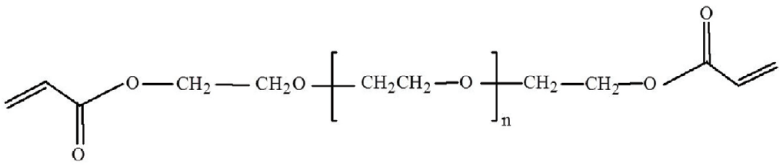
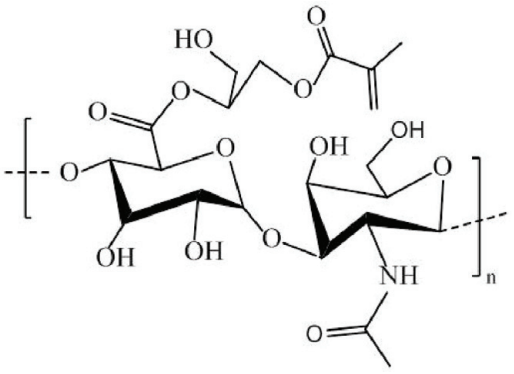
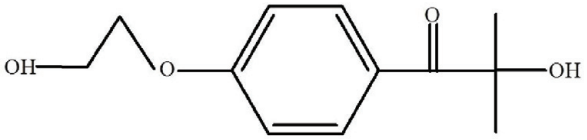
SUMMARY

Synthesis of materials and structures based on biostable and bioresorbable polymers - one of the important directions of modern biomedical materials science. Later these structures can be used for drug delivery or tissue substitution therapy sections or local organ damage. Chitosan is widely used for preparing scaffolds for regenerative medicine due to its ability to enzymatically bioresorption and high affinity to animal cells. One of the key characteristics of tissue-engineering structures are the optimal structures scale and the possibility of varying the 3-D architectonics of such objects. The structures scale could be varied by the method of polymer structuring. As an example, one of the methods of forming of three-dimensional microstructures, providing high spatial resolution is a method of two-photon polymerization or microstereolitography based on the effect of two-photon absorption. The development of a method of two-photon polymerization, which allows to form structures with high spatial resolution is a method of quick stamping or micromolding. Creating structures by traditional one-photon laser stereolithography is also a very promising method for creating three-dimensional structures. The low resolution of the method is compensated by higher productivity

1. Materials

Components of photopolymerizable compositions (PPC) are presented in Table 1.

Table 1. Components used for PPC

	Name	Structure
Main components of the reactive polymer system	Poly[(1 → 4)-2-amino-2-deoxy-β-D-glucose] (chitosan)	
	Allylchitosan	
	Graft copolymers of chitosan with polyvinyl alcohol (chitosan-PVA)	
	Graft copolymers of chitosan with oligo(D,L)-lactide	
Components used as cross-linker	Polyethylene glycol diacrylate (PEG-DA)	
	Hyaluronic acid-glycidyl methacrylate (HAGM)	
Photoinitiator	Irgacure 2959	

All chitosan copolymers were obtained by the original solid-state method in Enikolopov Institute of Synthetic Polymer Materials in Prof. T.A. Akopova group.

Chitosan was prepared by the solid-state method from the chitin of crab shells. The molecular weight of chitosan was 40–50 kDa, and the degree of acetylation was 0.30.

Allylchitosan was prepared using the solid-state method by reacting chitosan with allyl bromide in the extruder [1,2]. In a study used chitosan with varying degree of substitution (DS) of its functional fragments allyl groups:CHT-A1 = 0.1, CHT-A2 = 0.15, CHT-A3 = 0.2, CHT-A4 = 0.25, CHT-A5 = 0.5.

For the solid state synthesis of the **graft copolymers of chitosan with polyvinyl alcohol**, chitin and polyvinyl acetate (PVAc) were used as the reactants, whose deacetylation during the shear deformation of solid reactive mixtures for producing graft copolymers [2].

Graft copolymers of chitosan with oligo(D,L)-lactide. The chemical structure of the main characteristics of the copolymers are shown in Tables 1 and 2 [3].

Table 2.Chitosan-g-oligo(D,L-lactide) copolymer's macromolecular characteristics.

*DA - degree of acetylation; DD-degree of deacetylation; DS - degree of chitosan amino group substitution; PD - average polymerization degree of the side D,L-lactide chains

Sample	DA*	DD*	DS*	PD*
CL_1/0.5	0.1	0.71	0.19	3.0
CL _1/1		0.49	0.41	4.1
CL _1/3		0.53	0.37	9.7

Hyaluronic acid-glycidyl methacrylate. The chemical modification of hyaluronic acid was carried out in Hannover Laser Centre in a laboratory under the direction of Prof. B.N.Chichkov. Maximum degree of substitution of the product obtained is 60%[4].

2. Method of preparation and selected PPC compositions.

The optimum ratio of PPC components have been chosen and methods of PPC preparation to create three-dimensional structures by methods of micro-and macrostructuring using laser emmiting have been developed by us.

For photosensitive compositions were prepared 5% solutions of chitosan and its copolymers in 4% acetic acid (or in the case of compositions based on chitosan-g-oligo(D,L)lactide copolymers solutions were prepared in water). Next, the insoluble fraction was separated by centrifugation, after which the solution was decanted and filtered through a membrane. To form matrices by **method of 2PP** filtrates were placed in a evaporative weighing bottle where solutions were evaporated to a gel state. For PPC obtaining concentrated solutions (~ 20 wt.%) were mixed with an aqueous solution of Irgacure 2959 and stirred for 24 hours. We also examined the effect of adding in photosensitive composition of PEG-DA (2000 Da) and HAGM.

For the method of **stereolithography** and **micromolding** in 4.5wt% allyl chitosan solutions Irgacure 2959 photoinitiator have been added, mixing the solution is made within 2 hours. After PEG-DA added (700 Da), the composition is allowed to mix for 2 days.

3. Structuring of tissue-engineering scaffold

3.1. Two-photon polymerization (2PP)

For each PPC spectrophotometric analysis was carried out before the structuring. The absorption bands of used copolymers are in the field of up to 500 nm, intensive absorption band with a maximum at a wavelength of 280 nm refers to the photoinitiator, which indicates suitability for microstructuring by two-photon polymerization (Figure 1) [5].

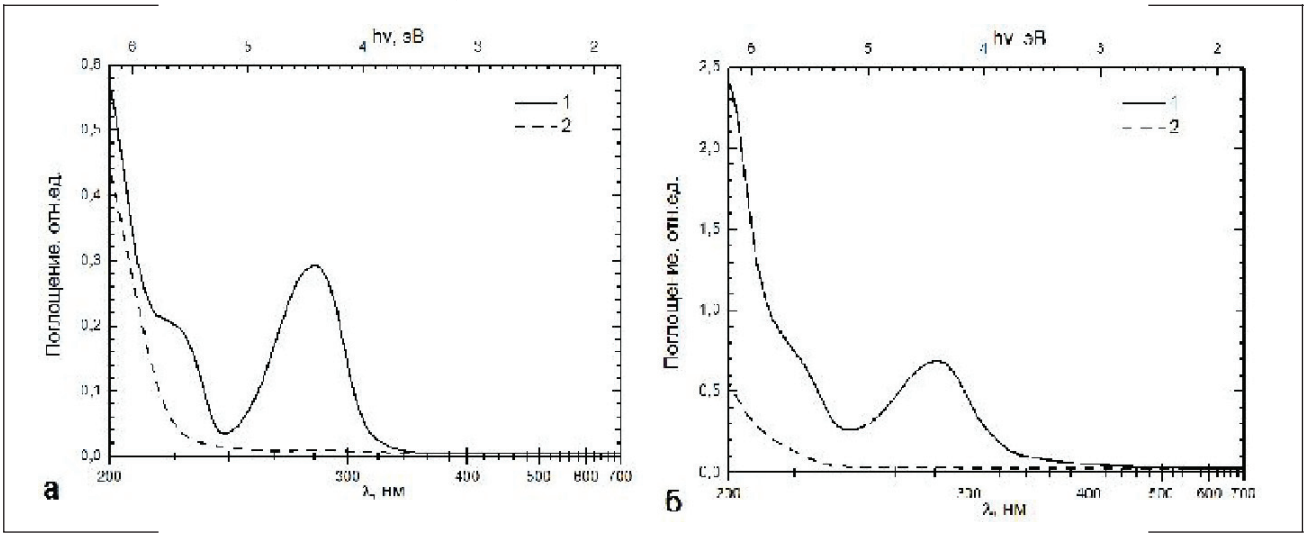


Fig.1. The absorption spectra of:
a) 1 - initial allyl chitosan with PEG-DA,
2 - composition of allyl chitosan,
PEG-DA and Irgacure 2959;
b) 1 - initial chitosan with HAGM,
2 - composition of chitosan, HAGM and
Irgacure 2959

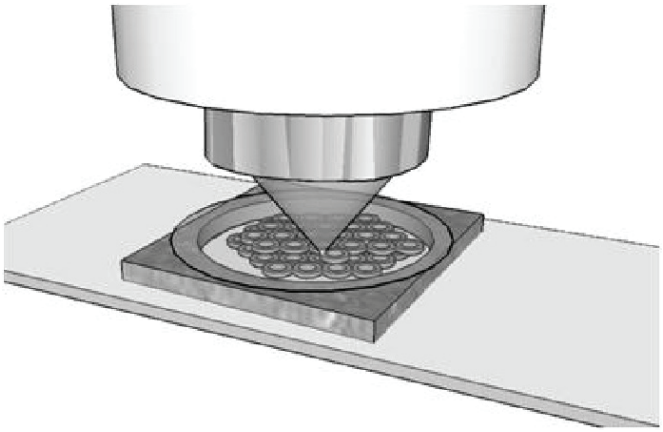


Fig.2. Schematic illustration of the structuring by 2PP

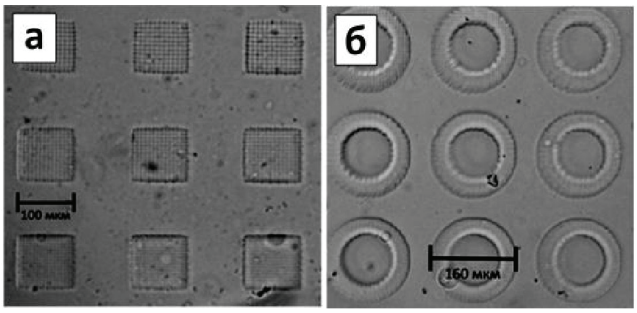


Fig.3 Photomicrographs of arrays obtained by two-photon polymerization of chitosan-PVA (a) and allyl chitosan (b).

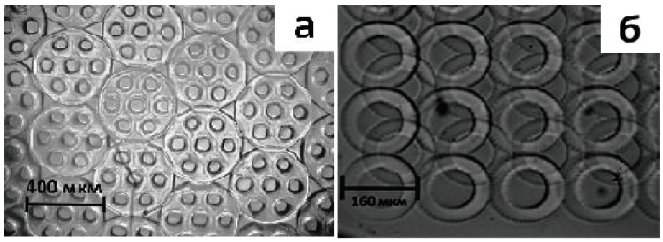


Fig. 4. Photomicrographs of three-dimensional structures of various models

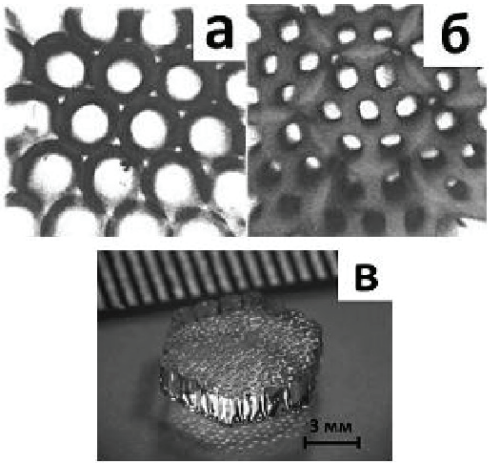


Fig. 5. 3D reconstruction of the washed hydrogel matrices (a, b); obtained scaffold based on allyl chitosan and PEG-DA after washing of the non-crosslinked material (в)

Samples of the photosensitive compositions were placed on a glass slide and were limited by spacer of crosslinked polydimethylsiloxane matrix (Figure 2). At the top cover glass was placed, through which the radiation took place. Cover glass prevented the drying of the composition and the crystallization of the photoinitiator.

First, for each sample the selection and optimization of 2PP-structuring parameters were carried out. With a scanner the number of vertical layers and the distance between them (from 5 to 10 microns) were changed, at the other axis the distance between individual ray passages (5 to 10 microns) was changed. For materials the speed of 2FP process and working laser power were selected: 50 - 150 mW, 5000 - 15 000 mkm/s. Fig. 3 shows the two-dimensional arrays of structural units, which were structured with various parameters [2].

Since the structures must be the network of macropores and pores, in turn, must be connected to each other to provide the cells ability to migrate through the matrix, to promote tissue growth throughout the scaffold, the size of the cylindrical structural units and their shape were varied while 2PP-structuring. Figure 4 shows two configurations used in works [2,5].

As a result, two-and three-dimensional structures have been formed on the basis of chitosan, allil chitosan, graft copolymer of chitosan and polyvinyl alcohol [2]. In the example copolymers of chitosan with oligo(D,L)-lactide with various grade of polymerization of graft chains was shown that the macromolecular characterization of the synthesized copolymers affect the holding microstructuring process: substitution degree increase in the amino groups of chitosan and the degree of oligolaktide polymerization in copolymers allows the formation of stable three-dimensional crosslinkings upon irradiation [3].

In our study, for each type of matrices developed an algorithm for washing out the non-crosslinked material. It contains a cyclic washing with aqueous ammonia, acetic acid and water. To check the completeness of washing, the hydrogel matrices were studied on an inverted microscope equipped with a confocal laser system (Figure 5)

3.2. Micromolding method [5]

In this study the technique of quick-forming matrices of biodegradable allyl chitosan on micromolding technology have been perfected. The method allowed to obtain scaffolds with a simple structure in quantities up to 10 pieces per day. The hydrogel was poured into a 3-dimensional matrix of polydimethylsiloxane fixed to the aluminium base (Figure 6), and then curing of the composition was initiated with a laser at a wavelength of 266 nm, the intensity of 2 mW/cm^2 for 5 minutes.

Model for the matrix has a hexagonal shape, which is a two-tiered array of cylinders, the diameter of a single cylinder ≈280 mkm (Figure 7).

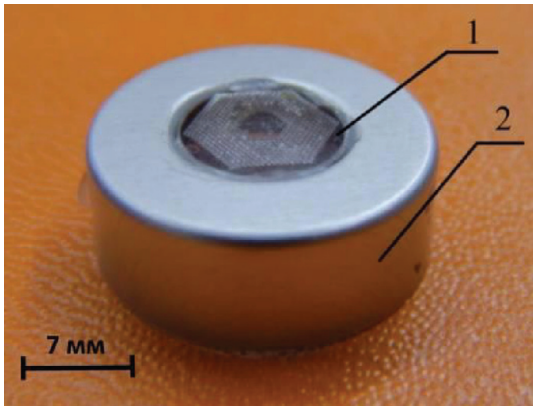


Fig. 6. The substrate for micromolding
1 - convex matrix of polydimethylsiloxane,
2 - aluminum basis.

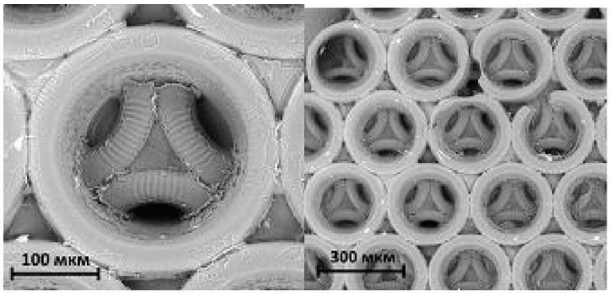


Fig. 7. Scaffolds obtained by micromolding based on allyl chitosan [5].

3.3. Laser stereolithography

All samples were prepared on an experimental model of laser stereolithography apparatus LS-120 . Layer thickness in growing samples was 200 μm. Structurization was performed using a HeCd-laser (wavelength was 325 nm, radiation power was 15 mW). We determined the layer formation rate based on the laser power and the technological parameters of the composition curing deduced from experiments: Ec=50 mJ/cm^2 (a parameter characterizing a threshold value of exposure dose for solid polymer film formation start) and Dp=0.15 mm (a parameter to characterize critical thickness of a film)[6].

CHT-A1 and CHT-A5 based matrices produced by laser stereolithography are structurally uniform material. The samples are in the form of crossed helixes (or two superimposed circles with centered beams, and a hole) or in the form of cylinders with slits (Fig.8). Under mild exposure original matrices recover their former shape[6].

Figure 8. Appearance of structured matrices; 1 scale mark = 1 mm

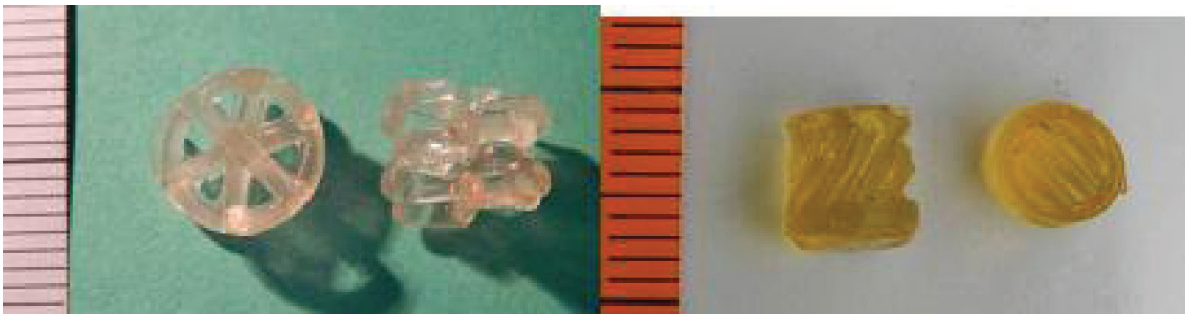
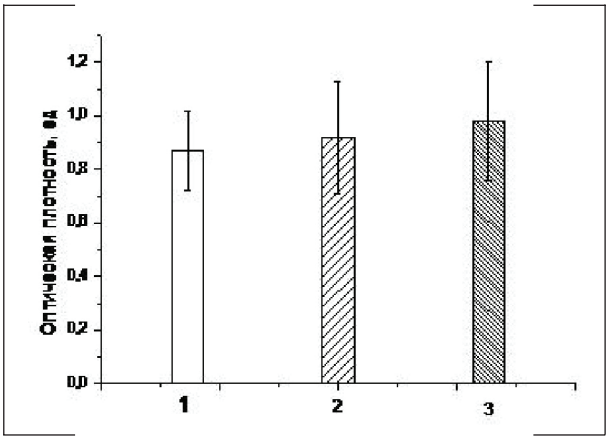


Figure 9. Metabolic activity of NCTC L929 line cells according to MTT assay in 48 h incubation of three-day extracts from materials: 1 — allyl chitosan; 2 — allyl chitosan + PEG-DA; 3 — on the cover glass surface



4. Biological research

4.1. Biocompatibility and biological activity of the chitosan-based composition[6]

Biocompatibility for materials based on allyl chitosan was studied in vitro using extractions and cell culture on the surface of the materials themselves. Partial replacement of chitosan amino groups by allyl groups (CT-A) and the introduction of polyethylene glycol diacrylate (PEG-DA) as a crosslinking agent were found not to reduce the material biocompatibility.

The metabolic activity determination of NCTC L929 cells using MTT assay showed that the samples under study to contain none water-soluble components toxic to mammalian cells (Fig.9).

The samples based on CT-A1 and CT-A1 with a crosslinking agent PEG-DA are biocompatible and are able to support adhesion, spreading and proliferative activity of human mesen-

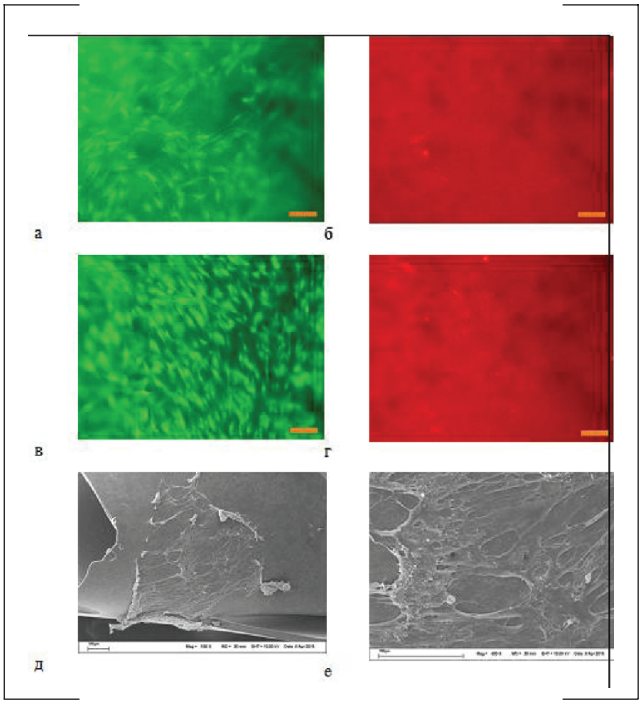


Figure 10. Appearance of human mesenchymal stem cells in incubation on the surface of allyl chitosan: incubation day 1 (a), (b); incubation day 7 (c)–(f). Cell staining Syto 9 (a), (c); propidium iodide staining of dead cell nuclei (b), (d); SEM microphotographs (e), (f)

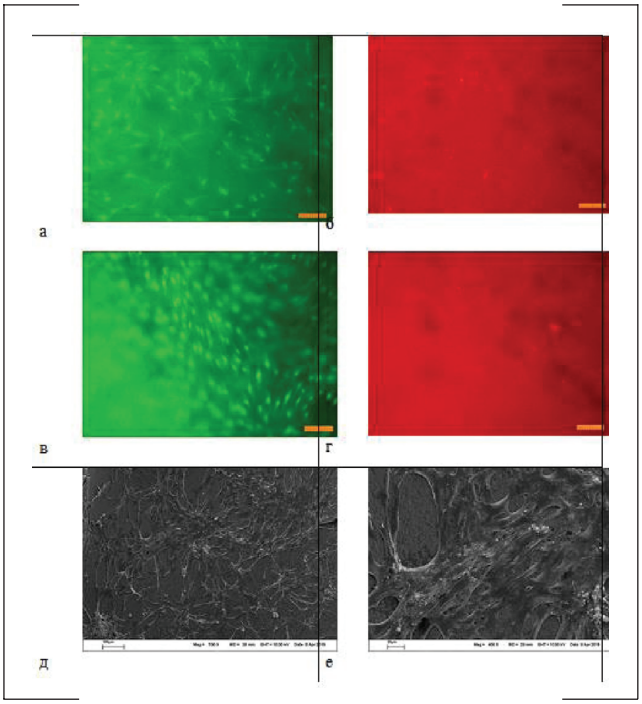


Figure 11. Appearance of human mesenchymal stem cells in incubation on the surface of allyl chitosan film + PEG-DA: incubation day 1 (a), (b); incubation day 7 (c)–(f). Cell staining Syto 9 (a), (c); propidium iodide staining of dead cell nuclei (b), (d); SEM microphotographs (e), (f)

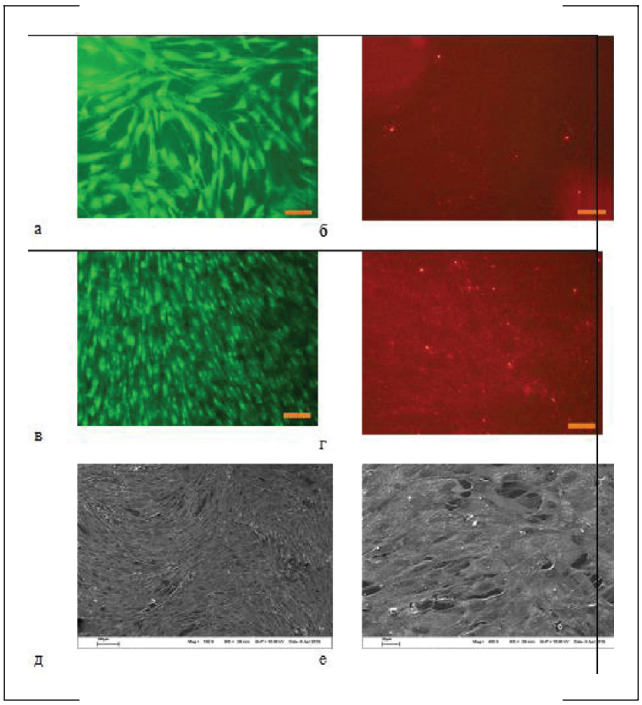


Figure 12. Appearance of human mesenchymal stem cells in incubation on the cover glass surface (control): incubation day 1 (a), (b); incubation day 7 (c)–(f). Cell staining Syto 9 (a), (c); propidium iodide staining of dead cell nuclei (b), (d); SEM microphotographs (e), (f)

chymal stromal cells (MSC), but have significant differences in the extent and nature of the expression activation of gene markers for osteogenic differentiation path.

The analysis of morphological traits and viability of human MSC cultured on the surface of CHT-A1 and CHT-A1 with PEG-DA demonstrated the cell death percentage not to exceed 1–2%. Cells spread and proliferated on the surface of both materials under study. The morphology of cells was no different from control, though the density of a cell monolayer on a cover glass on day 7 was significantly higher compared to that on polymer films (Figures 10–12).

To assess the effect of physicochemical characteristics of the materials on differentiating activity of human MSC we determined a phenotypic cell profile at different culture stages. The present study involved real-time PCR to analyze expression of 22 major genetic markers.

The study of the cell cultured on the glass and on the polymers under study showed the differences in expression activation degree of genetic markers of osteogenic differentiation on day 7 (Figure 13, a).

A longer cell culture (23 days) on the test materials slightly changed the gene transcription (Figure 13,b). On allyl chitosan samples only a few genes had a high expression level compared to the cells cultured on the cover glass. A control group, in general, showed the same transcription pattern of marker genes, though the majority of genes enhanced it significantly.

4.2. Compatibility of the nervous cells and structured biodegradable matrices[7]

For hydrogel matrices based on chitosan and HAGM defined toxic and adhesive properties and showed good compatibility with primary cultures of hippocampal.

It was found an intensive attachment to the hydrogel matrix of viable dissociated hippocampal cells at the end of the first day of culture.

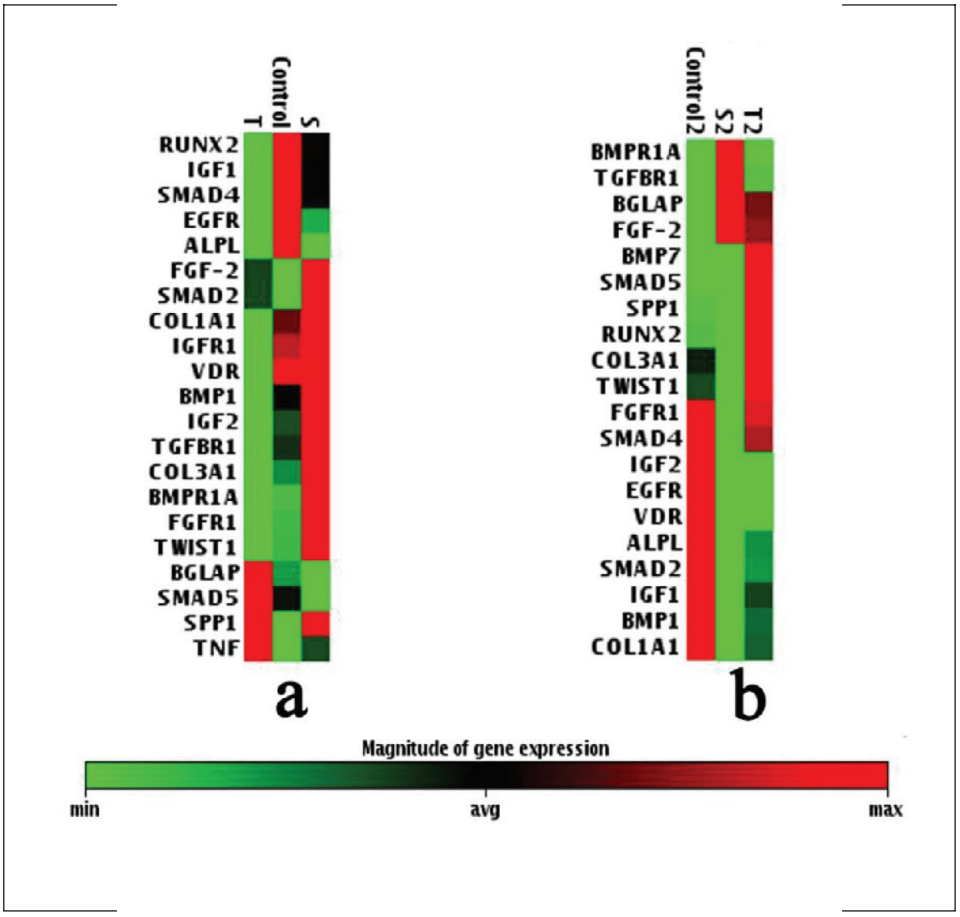


Figure 13. Gene expression levels in human mesenchymal stem cells cultured within 7 (a) and 23 days (b) on the surface of the materials: S and S2 — CHT-A1; T and T2 — CHT-A1 with PEG-DA; control — cover glass

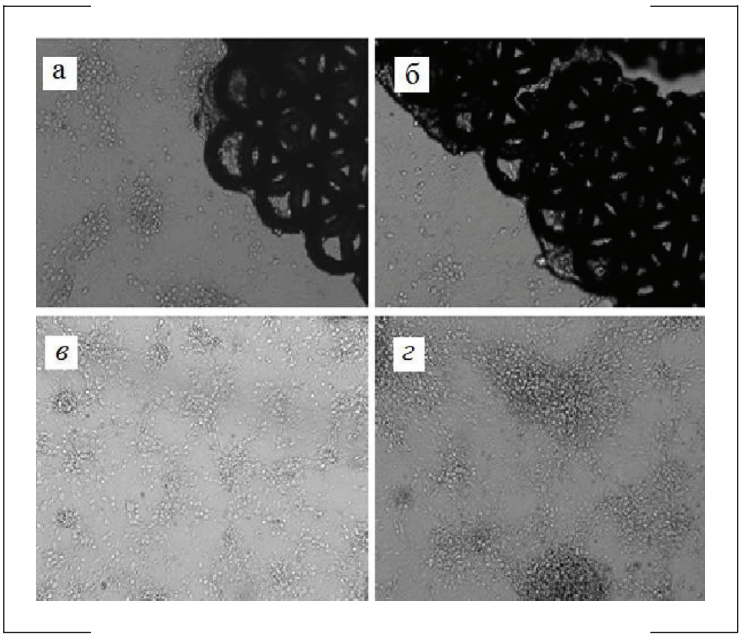


Fig. 14. Photomicrographs of dissociated hippocampal cells cultured on the hydrogel matrix based on chitosan (a and b DIV 14 and 30 respectively) and control (e, g, on a petri dish coated with polyethyleneimine)

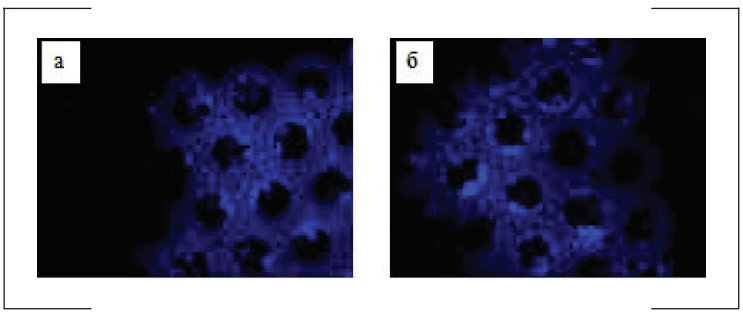


Fig. 15. Micrographs cultures of dissociated hippocampal cells cultured on a hydrogel based scaffolds for chitosan 14 (a) and 28 days (b) (stained by bis-benzimid)

Next it was observed shoot formation of nerve and glial cells on the surface of the matrix. This is indicative of activation of the processes of formation of the network structure.

Thus, it is shown that the chosen shape of a matrix conducive to the formation of morphologically full neuron-glial networks (Fig. 14).

Cytotoxicity of matrices was determined in vitro: uniform growth of cells throughout the matrix surface was maintained throughout the period of observation (Fig. 15).

It was found that the matrix material has a high affinity to cells of the nervous system (neurons and astrocytes). The proportion of dead cells in the culture did not exceed 3.5% for all the test cultivation stages (Fig. 16).

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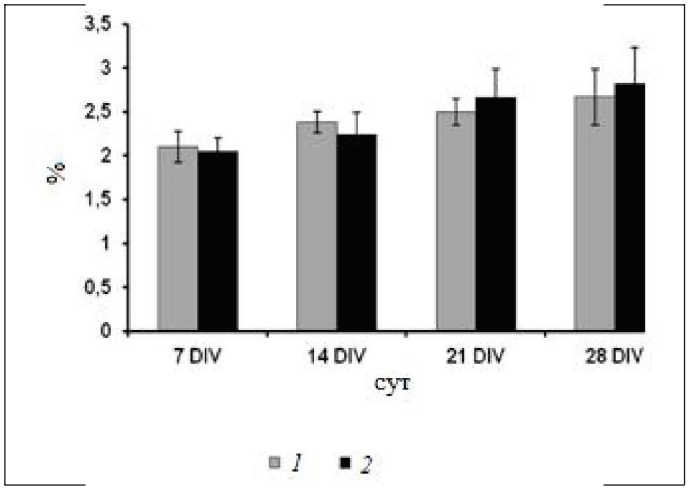

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Fig. 16. Change of a share (%) of dead cells in primary cultures of hippocampal for cultured on the glass (1, control) and hydrogel scaffolds based on chitosan (2)

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Effect of vacuum assistance on the void formation during liquid composite molding process

ABSTRACT

Effect of vacuum assistance during the impregnation stage of the liquid composite molding process on the void formation was experimentally studied. The dependence of the void content on the vacuum pressure was obtained. A model describing the results and the outlook were proposed.

KEYWORDS

Composites, liquid composite molding, voids.

ACKNOWLEDGEMENTS

This work was supported by Grant of Ministry of Education and Science of the Russian Federation (11.G34.31.0040) and Skoltech Partnership Program.

SUMMARY

Void formation during liquid composite molding (LCM) process is one of the challenges in manufacturing of composite parts. Voids significantly degrade shear and compression strength of composites. LCM involves the pressure gradient driven injection of liquid resin into the closed mold containing reinforcing fibers. Complex porous structure of the reinforcement can provide the gas entrapment and the formation of voids during the impregnation stage.

The effect of vacuum assistance to drive the resin flow on the void formation was experimentally studied. The transparent mold made of acrylic glass containing single layer of reinforcing fabric was used to simulate the LCM process. The designed mold allowed applying vacuum and compressed air pressure to inject the epoxy resin into the mold. The saturation curves were obtained at various applied vacuum pressure. The pressure gradient between the inlet and the outlet of the mold was keeping constant during all experimental tests. The volume fraction of voids in fabricated samples was estimated by facilities of optical microscopy and image processing techniques. The dependence of the void content on the vacuum pressure was obtained. A model for description of the obtained results and the outlook were proposed.

This work was supported by Grant of Ministry of Education and Science of the Russian Federation (11.G34.31.0040) and Skoltech Partnership Program.

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Investigation of boron delta doped layer growth

SCIENTIFIC ORGANIZATION

Institute of Applied Physics RAS

ABSTRACT

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KEYWORDS

CVD diamond, boron doped diamond, delta doping, diamond electronics.

SUMMARY

Attention to diamond as an electronic material is receiving international attention due to the improvements in the growth of synthetic diamond by both chemical vapor deposition (CVD) and high pressure high temperature (HPHT) techniques. Diamond offers significant advantages over other semiconductor materials due to its high electrical breakdown strength, high carrier mobilities, high thermal diffusivity, and other exceptional properties. Diamond semiconductor devices will likely impact applications in high power, high frequency, high temperature, and/or harsh or corrosive environments.

In this paper, the research results on the boron incorporation into the single-crystalline CVD diamond during the growth of the delta-doped layers are presented. Investigations were made on a new type of CVD reactor designed for growth of delta layers inside the diamond [1]. The reactor consists of a cylindrical cavity resonator with a quartz tube placed inside, in which laminar gas flow without vortex is maintained. The plasma is created in the reactor by the magnetron with 2.45 GHz frequency. Main features of the new type reactor are the following: (a) use of fast switching of feed gases flow, (b) reactor design, allowing creation of a laminar flow of gases. This approach allowed us to obtain heavily boron doped thin layers and to implement two-dimensional hole “gas” in diamond with high mobility and hole concentrations. Boron concentration in the delta layer and the doping profile was determined by SIMS method. As the result of experiments we found the optimal diamond deposition regime which allows to obtain doped delta layers with thickness of 1 - 2 nm with concentrations of boron greater than 10^{20} cm^{-3}. Such thin doped layers are highly desirable for the development of diamond-based field-effect transistor and other next generation electronic devices.

[1] A. L. Vikharev, A. M. Gorbachev, M. A. Lobaev, et. al, Phys. Status Solidi RRL, 1–4 (2016) 016) / DOI 10.1002/pssr.201510453

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In situ and operando studies of active phase in supported palladium nanocatalysts

SCIENTIFIC ORGANIZATION

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ABSTRACT

In a number of hydrogenation reactions, palladium nanoparticles may undergo a transition to the hydride or the carbide phase, which affects the catalytic properties. In the current work, we determine the structural evolution of an industrial Pd/C catalyst in the presence of hydrogen and acetylene by means of in situ X-ray absorption spectroscopy and X-ray powder diffraction. We observe reversible hydride phase formation and irreversible formation of the carbide phase. The near-edge structure of the absorption spectra (XANES) plays the key role in distinguishing between hydride and carbide phases. We show that the presence of hydrogen and carbon atoms have a direct effect on the near-edge region which is reproduced by theoretical simulations performed in the Monte-Carlo approach.

KEYWORDS

Palladium, catalysis, xanes, exafs, xrd.

ACKNOWLEDGEMENTS

Author acknowledge Mega-Grant of Ministry of Education and Science of the Russian Federation (14.Y26.31.0001) for funding the research.

SUMMARY

Metal nanoparticles play an important role in catalysis. For hydrogenation of hydrocarbons, such as alkynes and alkenes, palladium is recognized as the preferred catalyst. In reaction conditions, palladium nanoparticles may undergo phase changes to hydride and carbide phases, whose natures affect the catalytic properties. Therefore, determining the hydride and carbide formation during a catalytic process becomes an important problem, also relevant to industry. Being a subject of numerous theoretical and experimental studies, palladium hydride is one of the most-studied metal hydrides. In contrast to the hydride, the structure and properties of the carbide phase are still under discussion. The aim of the current work is to present a systematic approach for in situ and operando investigation of the formation of hydride and carbide phases in an industrial palladium-based catalyst under realistic working conditions.

The formation of both hydride and carbide phases is accompanied with an expansion of the palladium lattice, which can be followed by X-ray powder diffraction (XRPD) and extended X-ray absorption fine structure (EXAFS). EXAFS is an element-selective technique and demonstrates high sensitivity to the local structure changes, such as bond distances and coordination numbers of the absorbing atom. In the case of the palladium containing material, whose K- absorption edge is 24357 eV, hard X-rays can be easily applied to perform in situ and operando experiments. One should take into consideration that both EXAFS and XRPD are least sensitive to light atoms, such as carbon and especially hydrogen, due to their low scattering amplitudes compared to palladium. Thus, palladium hydride and carbide phases are observed by these techniques only indirectly, via Pd-Pd distance elongation or lattice expansion.

X-ray absorption near-edge structure (XANES) include a part of the absorption spectrum up to 30 – 50 eV above the absorption edge. It was shown that the formation of palladium hydride directly affects the shape X-ray absorption near edge structure due to mixing of unoccupied states of hydrogen and palladium. This makes XANES a promising tool for in situ investigation of palladium hydride and carbide formation, because unlike EXAFS and XRPD this method is sensitive to the presence of light atoms. For the first time, we have reproduced the changes in XANES by theoretical simulations applying Monte-Carlo approach.

In the presence of hydrogen the first near-edge peak at 24369 eV becomes narrower and is shifted by 1 eV to lower energy. Formation of palladium carbide leads to a broadening of the same peak and shifts it by 1 eV to higher energy. This opposite behavior of XANES spectra during hydride and carbide formation is more pronounced in the difference spectra and provides us a method to discriminate between the two phases under hydrogenation reaction conditions. To test this thesis we investigated the system sending at 100 °C a mixture of 650 mbar of hydrogen and 350 mbar of acetylene. Comparing the XANES spectrum collected under hydrogenation reaction conditions with those obtained sending at 100 °C the pure reagents separately (100 and 600 mbar of H2 or 1000 mbar of C2H2) we can conclude that hydride phase is formed, having a similar composition to that obtained sending 600 mbar of pure hydrogen at the same temperature.

In summary, we have demonstrated a scheme to obtain structural information on supported palladium nanoparticle relevant in catalysts by applying in situ and operando X-ray absorption and powder diffraction techniques. Analysis of XANES spectra allows determining whether hydride or carbide phase is formed in the nanoparticles. Possibility to extract this information from XANES becomes extremely important in the cases, when the catalyst is exposed to a mixture of gasses, and the type of the phase (carbide or hydride) cannot be predicted in advance. In addition to the type of the phase determined from XANES, and interatomic distance obtained from EXAFS, XRPD analysis gives quantitative information on the phase concentrations.

The described scheme of experimental measurements and analysis may be applied to investigate the structural evolution of supported metal nanoparticle catalyst during catalytic processes in operando conditions, such as hydrogenation of hydrocarbons and will allow correlating catalytic properties of the nanoparticles with their structure and phasing content.

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Investigation of the influence volume-surface hardening (VSH) on the tendency to corrosion of 20GFL steel used for cast parts of the railway transport

SCIENTIFIC ORGANIZATION

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ABSTRACT

In the paper the structure and mechanical properties of 20GFL steel used for the manufacturing the cast parts of railway vehicles (side frames, bolsters) after normalization and volume-surface hardening (VSH) have been studied. A new method of corrosion testing for 20GFL steel after a volume-surface hardening is suggested.

KEYWORDS

Railway transport, corrosion resistance, steel, volume-surface hardening, martensite.

ACKNOWLEDGEMENTS

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SUMMARY

Cast parts of railway transport made of 20GFL steel are subjected to heavy loads due to working in harsh climatic conditions. So, an actual issue is to improve the operational reliability of critical parts of rolling stock of the railway transport by providing high mechanical properties of the steel used for producing it. A promising method of steel hardening is a method called volume-surface hardening (VSH). VSH includes heating parts in the shaft furnaces, holding and cooling in the fast-moving stream of water which allows to carry out the hardening of the surface layer by producing martensite and also the hardening of the core section of the working parts at once. However, VSH influence on corrosion behavior of steels has not been investigated yet. In this regard, the purpose of the work is the study of the structure, mechanical properties and corrosion resistance of steel 20GFL after normalization and VSH; development of methods of corrosion testing of the samples of the side frame rail transport after the volume-surface hardening

Tasks: 1. Qualitative and quantitative study of the microstructure of the 20GFL steel in the initial state (after normalization) and after the VSH 2. Measurement of the microhardness over the cross section samples 3. Development and approbation of the methods testing corrosion resistance 4. Comparison of tne tendency to corrosion of steel 20GFL in normalized condition and after the VSH.

Metallographic analysis showed that:

- Lateral frames fragments microstructure after normalization is a ferrite-perlite mixture with an average grain size of 20 ± 10 microns;

- VSH leads to the changes in the structure of the fragment thtouth the cross-section: there is a decarbonized layer of 100 ± 30 mm and then hardened zone consisting of martensite and troostite and then troostite, thin plate ferrite-cementite mixture of the troostite, decarbonized layer (in the direction from the outer edge of the sample to inner, respectively).

Changes in microhardness after VSH showed a gradient nature of the cross section of the frames, and micro-hardness measurement results are consistent with the results of microstructural analysis: a) after the normalization of the mean value of 150-200 HV; b) after the VSH - 200-500 HV, the maximum microhardness is in the hardened zone - 500 HV, corresponds to the minimum and decarbonized layer is 200 HV

Based on the results of metallographic analysis and microhardness analysis and analytical review of the literature on the corrosion of low alloyed and carbon steel were developed and tested the methods of corrosion of 20GFL steel in the atmosphere and salt spray samples cut from the side of the frame. The preliminary results showed no substantial corrosion resistance, depending on the type of heat treatment. In testing the samples in salt spray corrosion set different speed after normalization and AEs different structural domains: decarbonized layer corrodes faster than 2.9 times than the hardened layer with a structure troostomartensita.

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Real-time nanomanipulations for tribological measurements of nanostructures

SCIENTIFIC ORGANIZATION

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ABSTRACT

In this work an experimental method of real-time measurements of tribological and mechanical properties of nanoparticles (NPs) and nanowires (NWs) using nanomanipulation technique inside a scanning electron microscope is presented. Specially designed quartz tuning fork based force sensor enabled friction force registration for manipulated NPs. Static and kinetic friction of NWs were found by a “self-sensing” approach based on the strain profile of the elastically bent NW.

KEYWORDS

Nanowires, nanoparticles, friction, manipulation, strength, Young modulus.

ACKNOWLEDGEMENTS

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SUMMARY

Nanoparticles (NPs) and nanowires (NWs) are now among the most important classes of materials in modern applied science, as they have demonstrated remarkable properties and have number of promising applications. In particular, fabrication of nanoelectromechanical systems (NEMS) requires precise control over positioning and behaviour of the NPs and NWs in various environments. Thus, deeper understanding of their mechanical properties is demanded. Commonly used tool for mechanical characterization of nanostructures is atomic force microscope (AFM) that features high precision and stability of the results but lacks in situ visual guidance.

In this work an experimental method of real-time measurements of tribological and mechanical properties of NPs and NWs using nanomanipulation technique inside a scanning electron microscope (SEM) is presented [1]. Measurements are based on visually controllable manipulations of the nanostructures with a sharp AFM tip inside SEM using nanomanipulator.

Polyhedron and sphere-like metal (gold and silver) nanoparticles (NPs) were manipulated on an oxidized Si substrate to study the dependence of the static friction and the contact area on the particle geometry. To register the occurring forces a quartz tuning fork (QTF) with a glued sharp probe was used. Experimentally measured force is compared to static friction forces found by using various models. The effect of NP morphology on the nanoscale friction is discussed.

NWs of oxide materials (ZnO, CuO) are manipulated by a sharp tip and being elastically deformed. NW bending profile is preserved due to the balance between intrinsic elastic force, lateral friction force from the substrate and the force of external manipulator. The state of mechanical equilibrium is described with use of continuum mechanics based models and further employed to find frictional properties of the NWs.

In particular, maximal static friction force is estimated when nanowire is being pushed at one end and switches from partial to complete motion upon overcoming static friction [2]. Static friction from the bent NW state can be also considered via a crack-based model [3]. Kinetic friction is extracted from the profile of the nanowire being uniformly dragged at the midpoint. After being brought to rest after the manipulations, the nanowire causes redistribution of static friction force from the supporting surface which is calculated and compared with kinetic friction [4]. Finally, a strong dependence of static friction on surface roughness is described [5].

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ADDITIONAL INFORMATION

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Femtosecond laser pulse nanostructuring of sodium silicate glasses

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ABSTRACT

Self-assembled birefringent periodical nanostructures known as nanogratings were induced by a femtosecond laser beam in R2O-SiO2 glasses with 5, 10 and 15 mol.% R2O (R=Na, K) and compared with those in fused silica. Obtained nanostructures possess similar period but number of laser pulses required to form nanograting grew substantially with alkaline oxide content that is presumably results from relatively slow migration of alkaline cations required to induce birefringence.

KEYWORDS

Nanograting, femtosecond laser, alkali silicate glass, birefringence.

SUMMARY

Interaction between femtosecond laser pulses and oxide glasses provide different types of space-selective modification. Among them, self-assembled periodic nanostructures also known as nanogratings draw much attention due to their form birefringence similar to that of uniaxial negative crystals as they consist of periodic nanolayers with various density [1].Importantly, retardance and orientation of these birefringent structures depends on the pulse energy or number and orientation of polarization of the laser beam, respectively, and therefore can be controlled and predetermined optically. This feature together with the excellent thermal stability of nanogratings opens up the way to numerous applications requiring smart and durable patterning of microbirefringence inside the glass including polarization converters, holography and “everlasting” optical 5D-memory [2]. Several possible mechanisms of nanograting formation have been proposed [1,3,4] but this issue is still under debate.

Most of studies performed were focused on obtaining nanogratings inside fused silica. Recently, evidence for femtosecond laser-induced nanogratings has been observed in glasses other than SiO_2 including reports on nanogratings in GeO_2 glass [5], binary titanium silica glass (ULE, Corning) [6], and several multicomponent borosilicate glasses (BK7, Borofloat, Schott) [6]. However influence of chemical composition of glass on nanogratings formation is still unknown.

In the present work self-assembled nanostructures written by femtosecond laser beam (Light Conversion PHAROS SP regenerative amplifier, 1030 nm, 600 fs) are demonstrated in binary alkali-silicate glasses. Laser writing of nanogratings in R_2O-SiO_2 glasses with 5, 10 and 15 mol.% R_2O (R=Na, K) is shown in comparison with fused silica. A period of nanostructures in alkalisilicate glasses is about 0.2-0.3 μm and is similar to a typical nanograting period in silica glass. On the contrary, a number of pulses giving rise to nanogratings grows with increasing alkali oxides content reaching ~10^5 pulses which is a few orders of magnitude higher than in pure fused silica. Still the final retardance corresponding to the prolonged laser treatment when process of nanograting formation is close to saturation approaches to that of the silica glass obtained by laser pulses with the same parameters. Local chemical analysis performed by means of energy-dispersive X-ray spectroscopy detected that alkaline cations partially move outside the area directly exposed to the focused femtosecond laser beam. Thus rise of birefringence presumably correlates to migration of alkaline ions and a long time required to form a nanograting as compared to that in fused silica may be related to the time which it takes to complete their migration.

This study was financially supported by the ministry of Education and Science of the Russian Federation (grant 14.Z50.31.0009) and Russian Foundation for Basic Research (grant 16-03-00541).

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SCIENTIFIC ORGANIZATION

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Boron Nitride Nanomaterials: Current Status of Developments and Applications

ABSTRACT

This talk will give an introduction to the rich Boron Nitride nanotube/nanosheet/nanoparticle field, including the latest achievements in the synthesis, structural analyses, property evaluations and industrial applications, and presents the purpose and significance of this direction in the light of the general Nanomaterial/Nanotechnology developments.

KEYWORDS

Boron nitride, nanotubes, nanosheets, nanoparticles, chemical vapor deposition, spark plasma sintering, high pressure torsion, transmission electron microscopy.

ACKNOWLEDGEMENTS

The presenter is deeply grateful to the National Institute for Materials Science, “NIMS” (Tsukuba, Japan) and the National University of Science and Technology “MISIS” (Moscow, Russian Federation) for a continuous support of his research.

SUMMARY

Hexagonal boron nitride (h-BN) is a layered material with a graphite-like structure in which planar networks of BN hexagons are regularly stacked. As the structural analogue of a carbon nanotube (CNT), BN nanotube (BNNT) was firstly predicted in 1994, since then, it has become one of the most intriguing non-carbon nanotubes. Compared with metallic or semiconducting CNTs, a BNNT is an electrical insulator with a bandgap of ca. 5 eV, basically independent of tube geometry. In addition, BNNTs possess high chemical stability, excellent mechanical properties and one of the highest thermal conductivities among of materials on Earth. The same advantages are applicable to a graphene analogue - a monoatomic layer of a hexagonal BN. Such unique properties make BN nanotubes, nanosheets and various types of nanoparticles a promising nanomaterial in a variety of potential fields such as optoelectronic nanodevices, waveguides, functional polymer and light metal matrix, and ceramic composites, hydrogen accumulators, water cleaners, electrically insulating substrates perfectly matching the CNT and graphene lattices.

The presenter is one of the founders of the booming nano-Boron-Nitride world research, in which he is continuosly engaged since 1994 and is one of the most influential world researchers in the general field of nanomaterials and nanotechnolgy. Golberg is included into the top 150 world most cited material scientists on the Web of Science, while having more than 600 publications in the International

Journals, which yielded more that 25.000 citations and a Hirsh factor of 84, and over 100 Japanese and International patents. His numerous awards include 2005 Tsukuba Prize for his developments of nanomaterial syntheses, 2012 Thomson Reuters Research Front Award for his studies of inorganic nanotubes and nanowires, 2014 “Seto” Award from the Japanese Microscopy Society to the best electron microscopist in Japan over the year, and 2016 NIMS President Prize. In 2016 he was also elected as an Australian Laureate Fellow. Thomson Reuters nominated Golberg as a Highly Cited Researcher in the consecutive years of 2014 and 2015. At present, Golberg is a Nanotube Group Leader and a Principal Investigator within the World Premier International (WPI) Center for Materials Nanoarchitectonics (MANA) of the National Institute for Materials Science (NIMS) in Tsukuba, Japan, and a Full Professor of the University of Tsukuba. His current research focuses on nanoscale material electromechanical, thermal, optoelectronic and photovoltaic property analysis using developed by him and his group state-of-the art methods of *in situ* transmission electron microscopy.

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New method for analyzing systems of channels and cavities in crystalline porous materials

SCIENTIFIC ORGANIZATION

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ABSTRACT

In this work, we describe new method for analyzing of crystalline porous materials based on the Voronoi partition of the crystal space. We have applied our method for 231 structures from the Database of Zeolite Structures. The widest 3-, 2- and 1-periodic channels in the structures were found. Volume and surface area of the channels were calculated and the topologies of the channels systems were identified.

KEYWORDS

Crystalline porous materials, zeolite, Voronoi tessellation, pore analysis.

SUMMARY

The crystalline porous materials such as MOFs and zeolites have wide industrial application. These materials are actively used for catalysis [1], gas storage [2] and separation [3]. One of the most important characteristic of crystalline adsorbents and catalysts is the information about system of channels and cavities and their geometry and topology. Previously, various methods were proposed based on grid [4], Delaunay [5] and Voronoi [6] tessellation approaches for calculation of pore descriptors in crystal structures.

In this work, we describe a new alternative method for analyzing of crystalline porous materials. This method is based on the Voronoi partition of the crystal space. As shown in article [7] the Voronoi net formed by vertices and edges of the Voronoi polyhedrons can be successfully used to find accessible channels (for a spherical probe with given radius) and its characteristics.

The novelty of our method consists in the new algorithm for calculation of pore geometry.

We have applied our method for **231** structures from the Database of Zeolite Structures [8]. The widest 3-, 2- and 1-periodic channels in the structures were found. Volume and surface area of the channels were calculated and the topologies of the channels systems were identified.

The work was supported by the Russian government (Grant 14.B25.31.0005).

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Light-emission enhancement in nanostructured gallium alkali-germanosilicate glasses

SCIENTIFIC ORGANIZATION

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ABSTRACT

In the present work we have studied the early stage of phase separation in gallium alkali-germanosilicate glass samples subjected to controlled nucleation treatment and have revealed the correlation between heat treatment conditions, strongly influencing concentration and size of γ-Ga2O3 nanocrystals, and luminescence efficiency of the resulting glass-ceramics.

KEYWORDS

Transparent glass-ceramics; γ-Ga2O3; solar-blind UV converter, nanocrystals.

ACKNOWLEDGEMENTS

This work has been supported by the Ministry of Education and Science of the Russian Federation under Grant No. 14.Z50.31.0009 and by Grant MK-8807.2016.3.

SUMMARY

Glass-ceramics (GCs) with embedded nanocrystals (NCs) are one of the most promising material for photonic and optoelectronic applications. UV-excited light emission of Ga_2O_3-based GCs is of particular interest because Ga_2O_3 photoluminescence is accompanied by complete lacking of any excitation channel in the visible and near-UV spectrum. It permits the fabrication of solar-blind UV-to-visible converters based on GCs for monitoring UV-emitting events such as flames, electric sparks, and corona dispersions. The size of crystals in mentioned GCs is usually in the nanometer region. Thus, photoluminescence properties are expected to depend on the particle size. To fabricate GCs with optimal UV-to-visible conversion, data are needed about the relationships between nanostructure parameters (size, concentration) and luminescence efficiency.

In recent years Ga_2O_3-based silicate GCs doped with transition elements has been studied intensively due to their broadband near-infrared emission [1]. In this field, we succeeded in the preparation of material with promising luminescent properties, based on germanosilicate GCs with gallium-containing spinel nanocrystals [2]. Moreover, we described the thermal evolution of native nanoinhomogeneities in Ni^{2+}-doped Ga-containing alkali-germanosilicate, based on SANS data, high resolution electron microscopy and infrared photoluminescence spectroscopy [3]. Detected nanostructures were found to be responsible for the appearance of Ni-related near infrared luminescence with a band centered at 1300 nm and bandwidth exceeding 300 nm.

At present, data on light emission properties in the visible of undoped nanosized Ga oxides are mainly available for nanopowders and nanowires, or NCs in

colloidal solutions [4]. A large fraction of those results regard the β-Ga_2O_3 phase, whereas only few studies concern the metastable polymorph γ-Ga_2O_3. Only in a recent paper we describe the intrinsic light emission of γ-Ga_2O_3 NCs dispersed in glass matrices [5]. We have found a novel and unexplored effect of spatial confinement on the donor-acceptor pair (DAP) recombination process when the nanocrystal size becomes comparable with the donor Bohr radius, and not too a low number of acceptors occur in the single nanocrystal. This confinement of DAP recombination depends strongly on the size of γ-Ga_2O_3 NCs and can enhance NCs photoluminescence in the case of exactly balanced DAPs. Such a system could in principle be tailored by controlling the nucleation process, which in turn determines concentration and size of undoped γ-Ga_2O_3 NCs and the resulting luminescence efficiency.

Our data show that luminescence is influenced not only by NC size change, and consequent modification of NC number density, but also by acceptor formation and passivation of Ga vacancies. In such processes, the interaction between the nanophase and the glass matrix plays a key role, providing the conditions for the occurrence of NC nucleation, NC coalescence, and Li incorporation, with a balance that depends on the nucleation temperature. These findings give a new direction to design transparent GCs with enhanced luminescent efficiency of embedded wide-band-gap NCs.

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Effect of heat treatment on microstructure and tribological characteristics of the samples produced by the method of additive manufacturing

SCIENTIFIC ORGANIZATION

Kazan National Research Technical University named after A.N.Tupolev

ABSTRACT

The work established that the heating the samples to a temperature of 1050 C (1.5 hr exposure) obtained by direct application of the laser leads to increased wear resistance. Reduced strength is achieved through the provision of grain carbide phases. The structural zone formed during LMD. It was found that the cross-sectional structure of the samples consists of alternating columnar and small zones variously oriented crystals.

KEYWORDS

Direct laser deposition of the material, heat treatment, nickel alloy, microstructure, wear resistance, durability, strength.

ACKNOWLEDGEMENTS

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Advanced electric pulse consolidation methods of powder materials

SCIENTIFIC ORGANIZATION

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)

ABSTRACT

Technologies of field-assisted powder consolidation are studied and further advanced at the Key Laboratory for Electromagnetic Field Assisted Processing of Novel Materials at NRNU MEPhI. The object of research is the advanced technologies of spark plasma sintering, microwave sintering, high-voltage electric-discharge compaction, and magnetic pulse consolidation of powders. A number of the obtained theoretical and experimental results have been used in the development of new methods of consolidation of powder materials using electromagnetic fields.

KEYWORDS

Spark plasma sintering, microwave sintering, high-voltage electric-discharge consolidation, magnetic pulse compaction, powders.

ACKNOWLEDGEMENTS

The support of the Department of Science and Education of Russian Federation (Grant Contract 11.G34.31.0051) is gratefully appreciated.

SUMMARY

Emerging technologies of field-assisted powder consolidation are studied and further advanced at the Key Laboratory for Electromagnetic Field Assisted Processing of Novel Materials at Moscow Engineering Physics University. The object of research is the advanced technologies of spark plasma sintering, microwave sintering, high-voltage electric-discharge compaction, and magnetic pulse consolidation of powders. The availability of the laboratory allows MEPhI to actively participate in projects related to the creation of new materials (such as the Russian-Ukrainian joint research project “Development of Methods of Processing and Consolidation of Composites Based on Iron and Titanium Carbides and Borides by Highly Con-

centrated Energy Fluxes" (grant of the Russian Foundation for Basic Research and of the Ukraine National Academy of Sciences).

The laboratory equipment includes: 1) Materials Processing Equipment: Spark Plasma Sintering System model Labox- 625 and a unique system Labox-125VHD of spark plasma sintering with hybrid heating (Japan); system Impulse-BM for high-voltage consolidation of powder materials; magnetic pulse powder pressing system Impulse 8-1 (Russia); high-temperature vacuum tube and muffle furnaces; a unique system of hot-pressing with an additional source of direct current; high-temperature vacuum microwave system Hamilab V6; isostatic press; uniaxial presses; ball mills, automatic mixers and dryers; plasma sputtering unit; dip coater (USA); etc, 2) Auxiliary Equipment: molding press and glove box; grinding and polishing machines; cutting machines (USA, France); vibratory sieve shaker (Germany); ultrasonicator (USA), 3) Materials Characterization Equipment: dilatometer (Germany); metallographic optical microscope; digital scales; automatic helium pycnometer (USA); a universal mechanical testing machine; microhardness tester (Italy); laser particle size analyzer (Germany); DSC-TGA thermoanalyzer (USA).

A number of the obtained theoretical and experimental results have been used in the development of new methods of consolidation of powder materials using electromagnetic fields. The most important fundamental theoretical results include: the first method of direct multi -scale modeling of sintering has been developed; a conceptually new experimental approach of Multi-Step Pressure Dilatometry, which can be effectively used to determine the basic mechanisms of spark plasma sintering, has been elaborated; new, having no previous analogues, models of inter-particle heat balance in the processes of spark plasma sintering and high-voltage electric discharge compaction have been put forward; new and original ideas of the influence of the geometry of the inter-particle contacts on the spark plasma sintering efficiency have been proposed; the first fully coupled finite element model of the process of hot pressing, activated by Joule heating, has been developed; the world's first models of mass-transfer associated with densification and contact growth during microwave sintering under the influence of ponderomotive forces have been developed; original description of the physics of densification in the process of magnetic pulse compaction has been introduced. New constitutive models of spark-plasma sintering taking into account thermal and non-thermal mechanisms of material transport are explored based on fundamental experimentation and computer simulations. Ultra-rapid field-assisted break-through consolidation technologies are developed for the processing of hard and super-hard materials. New technological routes of the fabrication of functionally structured powder components, including ODS steels and mono-nitride powders by spark-plasma sintering are established. Novel multi-scale thermo-mechanical model of high-voltage electric discharge consolidation of conductive powders is developed. New hybrid field-assisted sintering techniques are elaborated.

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Compaction of zirconium powders by high voltage electric discharge consolidation and spark plasma sintering

SCIENTIFIC ORGANIZATION

National research nuclear university «MEPhI»

ABSTRACT

This work presents the results on the comparison of two sintering techniques: HVEDC and SPS. Features of the consolidation processes of zirconium alloy powders with particles of various shapes have been identified. The average particle size of the powder was 250 μm. The optimal processing modes enabling the fabrication of high-density samples have been determined. The mechanical properties of samples have been measured by Vickers hardness test. A comparison of the results had been discussed according to data of mechanical tests and microstructure investigations.

KEYWORDS

Field-assistant consolidation, spark plasma sintering, zirconium, powders.

ACKNOWLEDGEMENTS

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Combining nanocalorimetry and synchrotron nano-focus X-ray scattering to address fast structure formation processes

SCIENTIFIC ORGANIZATION

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ABSTRACT

An original experimental setup developed in our laboratory in the frame of the Mega-Grant project will be described. It combines nano-focus X-ray scattering and ultra-fast calorimetry, or nanocalorimetry, and is designed for simultaneous in-situ measurements of structural and thermodynamic parameters of nano-sized samples. Examples of applications of the setup include inorganic and nanostructured hybrid systems. For the first time, in-situ nanocalorimetry / X-ray scattering experiments are reported for heating ramps at a rate of several thousands of degrees per second.

KEYWORDS

Nano-focus X-ray scattering, ultra-fast calorimetry, semicrystalline polymer, polymer crystallization.

ACKNOWLEDGEMENTS

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SUMMARY

Extending conventional methods of physical-chemical characterization to smaller and smaller sample size is crucial for the application fields where the amount of available material is limited. For example, in pharmaceutics the cost of a new material synthesis can be prohibitive and, therefore, very small sample size is often

all what is available to study the necessary structural and thermal characteristics. Handling very small sample sizes is also required in studies of thermal behavior of energetic materials that produce a deflagration reaction, with all the associated risks in terms of safety. However, to significantly shift the scale of the sample sizes downwards, it may be necessary to introduce completely new ideas into the instrumental design. For example, extending differential scanning calorimetry (DSC) for probing minuscule sample amounts has dramatically changed all the implementation of this conventional technique. The advent of nanocalorimetry has become possible because of the development of Si-based technologies allowing fabrication of novel MEMS-type sensors suitable for such sample sizes. One of the first commercially available MEMS sensors produced by the Xensor company (TCG 3880) reached a sensitivity of 1 nJ.K-1 and a time resolution of 5 ms [1]. The approaches toward quantitative nanocalorimetric experiments were developed further by M. Merzlyakov [2] and C. Schick [3].

The active area of the nanocalorimetric sensor is fabricated on a thin free-standing membrane of silicon nitride, a material with a relatively low thermal conductivity. Heating of the nanocalorimetric sensor can be realized by applying voltage on specially designed heating resistances. The sensor temperature can be measured using an array of thermopiles assembled on the active area. Since the heating and cooling rates that can be employed are much higher than in the classical DSC, much smaller samples become amenable to study as compared to the classical DSC. Although the advent of nanocalorimetry has significantly broadened the field of applications of the technique, a combination of calorimetry with other methods of physical-chemical characterization remains very attractive: the calorimetric measurements alone cannot always reveal the mechanisms of complex processes occurring in the material.

In our previous works, we described our custom-built nanocalorimetric accessory allowing for a combination of nanocalorimetry with other characterization techniques such as optical microscopy in reflection and transmission [4,5]. One of main advantages of our instrument compared to the commercial nanocalorimeter (i.e., “Flash DSC 1” from Mettler-Toledo) is that its design is fully open for integrating it into other experimental platforms. This is critical if one plans to make this accessory compatible for example with micro- and nano-focus synchrotron X-ray diffraction in transmission. The first successful in-situ measurements using nanocalorimetry and nano- and micro-focus X-ray diffraction, which has been developed in the frame of our Mega-Grant project conducted at the Moscow State University, were performed on metal micro-particles [6] and nanostructured hybrid materials [7].

In the present contribution, we report on the first application of a combined nanocalorimetry / nanofocus X-ray scattering accessory for in-situ studies of the structure formation processes in semicrystalline polymers. We also present the first in-situ measurements using a combination of fast calorimetry and fast X-ray scattering realized with a brand new family of X-ray detectors. The X-ray acquisition rate record achieved for the moment for a typical polymer sample deposited on a nanocalorimetric sensor is as fast as 1 ms/ frame. This rate makes it possible for example to perform real-time fast heating/cooling experiments at rates up to 10,000 °C/s with simultaneous recording of the sample heat capacity. As will be shown in the presentation, such combination can be valuable in analyzing the details of the microstructural evolution during fast heating of the semicrystalline polymers. In particular, based on the results of combined nanocalorimetry / nanofocus X-ray scattering experiments, we were able to revisit the long-standing issue of the multiple melting behavior in semirigid-chain polymers [8]. Moreover, the developed combination of nanocalorimetry / nanofocus X-ray scattering allows us to analyze such fundamental features of polymer crystallization as its departure from equilibrium, which has important implications for understanding of the polymer crystallization thermodynamics.

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Combined ab-initio and topological approach for prediction of new materials for energy storage

SCIENTIFIC ORGANIZATION

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ABSTRACT

Modern technologies demand high-efficiency portable electric energy sources. The development of new materials for energy storage is very urgent task (taking into account the lack of lithium for large-scale application). We apply combined topological and ab-initio approach to predict new functional materials for solid state batteries. Here we present our recent results of DFT and topological calculations of different types of ion-conductive materials. The combination of topological and quantum-mechanical investigations allows to achieve the most comprehensive results.

KEYWORDS

Solid State Physics, Material Modelling, Solid State Batteries, DFT, Ionic conductivity.

ACKNOWLEDGEMENTS

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SUMMARY

The existing technologies demand to portable energy sources. Such sources should be safe, cheap, effective, compact and environment-friendly. During past two decades lithium-ion batteries provide impressive advances in mobile electronics and electric vehicles [1,2]. This technology's jump was possible due to remarkable properties of lithium-conductive materials, especially high energy density. At the same time, the researchers have been exploring a lot of new materials for energy-storage applications and a routes to increase solid-state battery performance (specific energy, cyclability etc.) [3-8]. From the other side, battery safety stays a cornerstone for designing of new materials. One more reason affected on the searching is a lack of lithium for large-scale applications (for example, grid-based energy storage system for renewable energy sources) [9]. This leads to active exploring of sodium, potassium, aluminium-conducting materials as a promising candidates for replace Li-conducting ones.

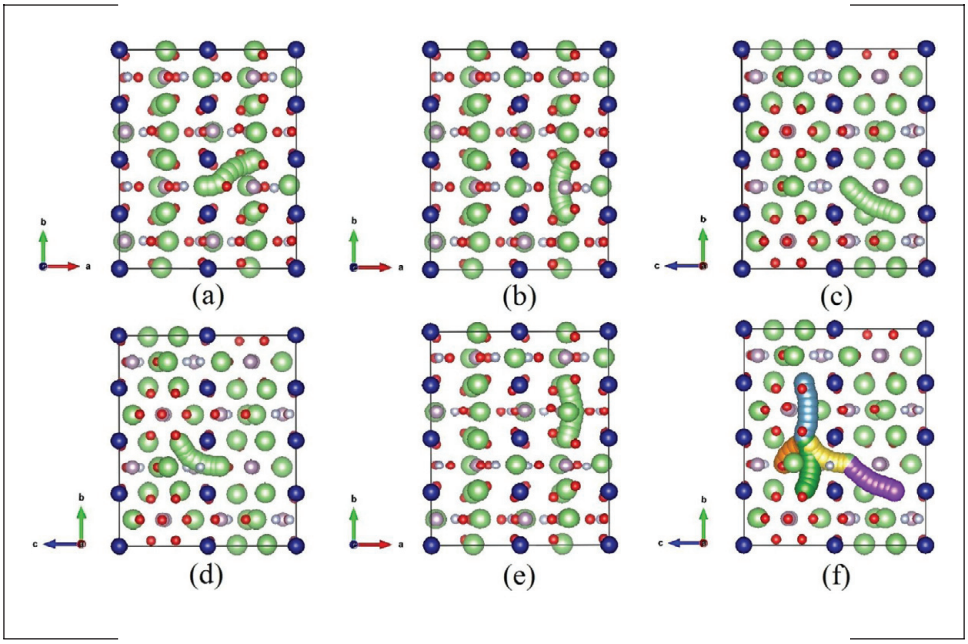
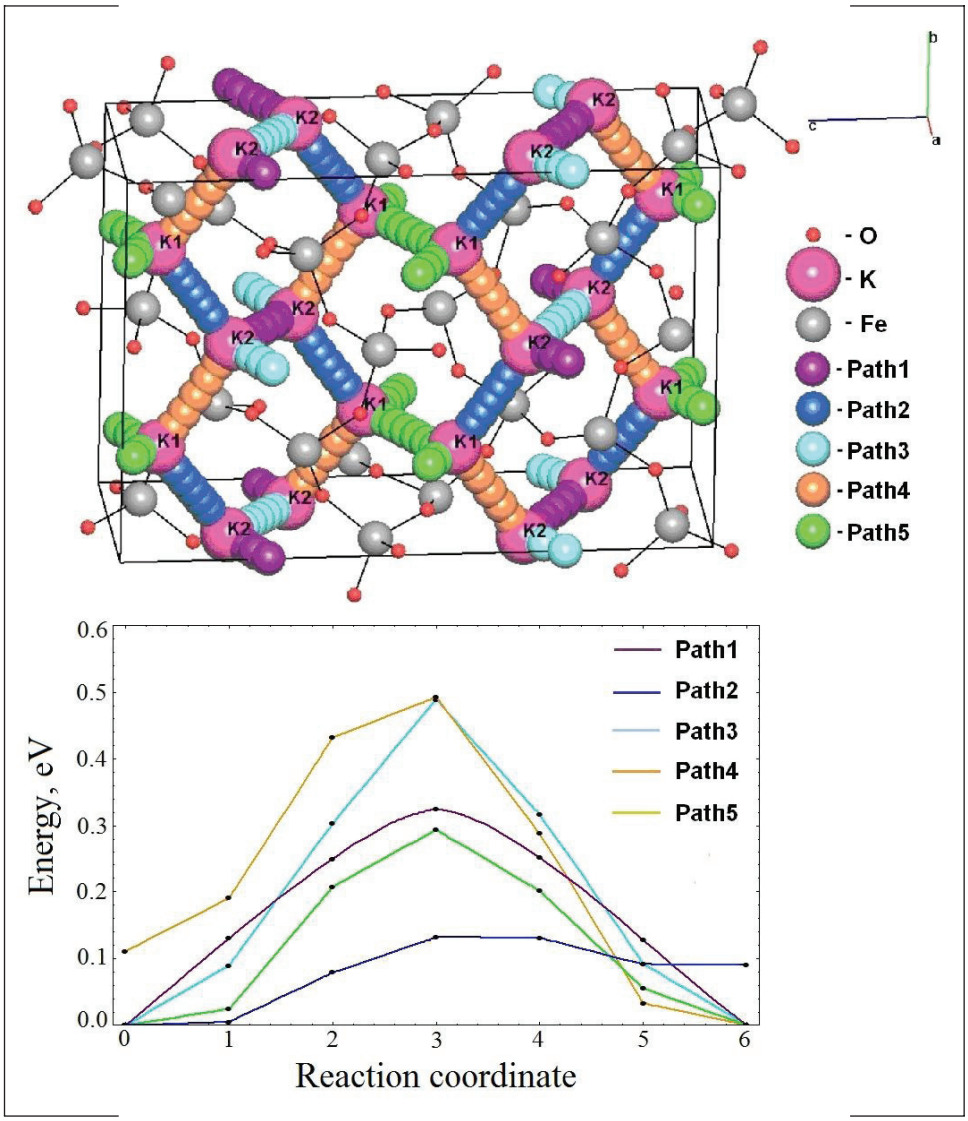


Figure 1. Curved trajectories for Li ion migration in Li_2CoPO_4F according to NEB calculations. (a),(b),(c),(d) and (e) panels corresponds to five non-equivalent paths. Panel (f) represent all five channels in the supercell.

Figure 2. Curved trajectories for K ion migration in $KFeO_2$ according to NEB calculations. Top panel represents all non-equivalent paths (marked by different colors). Bottom panel represent DFT results for activation energy values for each path.



The modern computational methods provide an excellent opportunity for numerical investigation of materials. Density functional theory – based methods (also called as first-principles, or ab-initio methods) are able to predict a key properties of materials, including ion mobility, electronic structure, cell voltage, thermal stability and voltage profiles [10]. DFT-based calculations open so called «high-throughput» searching when a lot of materials are explored computationally without resource-consuming experiments. But, instead of resource-consuming experiments, some DFT calculations demands processor time-consuming calculations. To minimize such calculations, we divide analysis of conductivity on two steps: i) initially we perform fast topological analysis of selected structures to determine the possibility of migration and, ii) we perform DFT calculations for the structures which have the appropriate channels for migration, according to step (i).

Here we used Vienna Ab-initio Simulation Package (VASP) [11] as the basic code for DFT calculations. To compute activation energy barriers, nudged elastic band (NEB) method [12] was used as it is implemented in VASP package. Topological analysis of possible migration channels was performed by using the ToposPro geometrical tiling analysis [13].

The following compounds were investigated using combined topological and DFT-based approaches: $LiCoO_2$, Li_2CoPO_4F, $LiVPO_4F$, $KFeO_2$, NaFePO4, $NaMnAsO_4$, $NaFeVF_7$, $Al_2(WO_4)_3$, $AlFe_2O_4$ and some others. The migration maps, activation energy barriers and electronic bands were computed. Usually structures have a few possible migration pathways and we calculated the activation energies for each of them. An examples of such calculations are presented at Figures 1 and 2.

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Kenny Jose

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Nanotechnology of Advanced Composite Materials

SCIENTIFIC ORGANIZATION

Institute of Macromolecular Compounds Russian Academy of Sciences

KEYWORDS

Nanotechnology, composite materials, processing.

SUMMARY

The control of the nanostructure and the addition of nanoparticles to polymers has led to structural and functional property enhancements in a number of polymeric systems as a material answer to continuous requirements from advanced industrial sectors. The availability of new nanoparticles with extraordinary properties (i.e. carbon nanotubes, graphenes, but also nanoclays, nanocellulose, metals and ceramics) have determined new and exciting possibilities for a continuous enlargement of polymer markets. However, the potentialities of these new materials are still strongly dependent on the development and scaling-up of reliable processing routes. So, the purpose of this report is to review the main processing approaches for nanostructured polymers and nanocomposites starting with a brief review of available nanoparticles and on their functionalization to promote a better polymer-particle interaction. Regarding processing, this review firstly addresses

the bottom-up approaches typically adopted for nanostructured polymers, blends and copolymers. Then, the different technologies required by the top-down processing of thermoplastic and thermosetting polymer matrix systems are reviewed. Finally, this report addresses the recent applications of nanostructured polymers and nanocomposites as matrices of advanced composite materials. In all cases, the main processing approaches and the main structural and functional properties characterizing these materials and their potential and current relevant industrial applications as aerospace, naval, automotive, cosmetics, bio-medicine (scaffold for tissue engineering, filling resins for prosthetic dentistry, etc.) and food packaging, among others, are specifically addressed.

Kiselev Evgeniy
PhD

Scaling of biodegradable polyhydroxyalkanoates synthesis technology in pilot production conditions

SCIENTIFIC ORGANIZATION

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ABSTRACT

On the basis of experimentally achieved and developed technical and technological parameters of biosynthesis processes the baseline data were obtained and the project was worked out for organization of pilot production of degradable polyhydroxyalkanoates (PHAs). The pilot line for production of polyhydroxyalkanoates was designed, equipped and commissioned, including the “Bioengineering” fermentation line (Switzerland), as well as the blocks for preparation of inoculum and culture media, isolation and purification of polymers.

KEYWORDS

Pilot production, baseline data, designing, procurement, equipment, material costs, process indicators.

SUMMARY

Implementation of a new technology in pilot production (PP) conditions is a necessary step for scaling and subsequent industrial production. Technology testing in PP conditions makes it possible to specify the physical and chemical parameters of fermentation process, to create a mass and energy balance, to develop a process procedure and to get batches needed to conduct a complex of required tests. The first domestic PP of polyhydroxyalkanoates (PHAs) was constructed and put into operation in January 2005 on the basis of Krasnoyarsk Scientific Center of the Siberian Branch of the RAS during the collaboration between the Institute of Biophysics SB RAS and the Biotechnology Department of the “BioKhimMash” JSC (Moscow) as part of the project of the International Science and Technical Center (ISTC) (Volova et al., 2006). The PP featured standard equipment of domestic production and non-standard equipment manufactured by those who implemented the project. The process was based on the technology using the bacterial strain Ralstonia eutrophus B5786 with the biomass and polymer yield up to 50 g/l and 80-85 %, respectively. The achieved production rates with regard to total biomass and polymer were 0.045 0.036 kg/hr (1). The studies carried out as part of the megaproject “Biotechnology of New Biomaterials” implemented under the supervision of the leading scientist, MIT professor Anthony John Sinskey (USA) (Resolution of RF government No 220 of April 9, 2010), as a result of which it was possible to significantly increase the efficiency of PHA biosynthesis due to the obtained strain of bacteria Cupriavidus eutrophus B-10646 able to synthesize PHAs with different chemical structures on various carbon sources, made it possible to proceed to the drafting of a new and more productive pilot production (PP).

Baseline data for the design of the pilot production of degradable polyhydroxyalkanoates (PHAs)

Based on the analysis of the obtained polymer synthesis results in different modes (autotrophic and heterotrophic), it was decided to choose for scaling the option implemented on more affordable glucose. As a result of the work conducted, it was possible to significantly increase the yield of polymers from 2 kg per cycle to

9.5 kg per cycle. More affordable glucose was used as a carbon substrate. The extraction time was reduced from 12 to 8 hours. The long process of settling was replaced by filtering, which reduced the time of oilcake separation from the extract to 8 hours. The pretreatment of biomass by a detergent solution made it possible to increase the degree of polymer extraction to 98.5%, as well as to avoid the formation of azeotropic mixtures, which made possible the regeneration and return of the solvents to the process. The obtained baseline data were the basis of the project of PHA pilot production and the choice of production equipment.

As a result of the complex research performed using the obtained strain C. eutrophus V10646 and optimization of PHA biosynthesis, certain indicators were achieved which were taken as a basis for drafting pilot production. In accordance with the developed project, the pilot production was equipped and commissioned including the “Bioengineering” fermentation line (Switzerland) and blocks for production of inoculum and growth media, isolation and purification of polymers. The pilot plant was put into operation. The achieved results of bioplastics biosynthesis at a final concentration of cells biomass in the culture C. eutrophus V10646 and polymer 110 ± 10 g/L and 85 ± 5% were, with regard to biomass and PHA, 1.7 and 1.4 g/l · hr, respectively, i.e. up to 500 kg of polymer/year. The pilot plant was put into operation, certified and is now successfully operating. The scaling of technology made it possible to produce experimental batches of polymers with different chemical structures in the amounts necessary to obtain specialized high-tech products (films, membranes, ultra-thin fibers, nano- and micro-particles, 3D carriers of drugs and cells). It facilitated the organization of regulated research and standardization of specialized polymer products. The pilot production is an educational base for training of graduate and post-graduate students in “Biotechnology”.

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ADDITIONAL INFORMATION

The study was carried out with the participation A.V. Demidenko, S.V. Baranovskiy, T.G. Volova.

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Fiber laser welding of metal materials

SCIENTIFIC ORGANIZATION

Kazan National Research Technical University named after A.N. Tupolev

ABSTRACT

The topic contains the list of ongoing and prospective work on the basis of the Regional engineering center “KAI-Laser” and the of Laboratory of Additive Manufacturing Technologies for laser welding. Described technological solutions designed to enhance weldability of dissimilar metals, aluminum alloys, steels. Presented promising directions of work for the different industries aviation and engineering. The review of foreign technology laser welding “flying metal.”

KEYWORDS

Fiber laser, laser beam welding, microstructure, mechanical tests.

ACKNOWLEDGEMENTS

The present research was conducted within the project under the resolution No. 220, contract No. 14z50.31.0023 with financial support of the Ministry of Education and Science of the Russian Federation. The authors are grateful to the Regional Engineering Center «KAI - LASER» for the opportunity to conduct experimental research.

SUMMARY

Laser welding (LW) is a promising method for joining metal materials. The main advantages of LW are: low heat input, high energy density, high speed of the process, the possibility of welding of large thickness in one pass, a high degree of process automation and control the laser power. The laser beam welding allows a similar materials and dissimilar. Various processing methods are used to obtain high-quality welded joint, such as: welding a defocused beam, the use of the beam oscillations, welding with “cold” filler material, welding with preheating defocused laser beam, etc.

At present, on the basis of the Regional Engineering Center “KAI-Laser” carried out the following works for laser welding:

- High speed laser welding (up to 100 mm / sec) of small thickness;

- Welding of aluminum alloys;

- Welding of copper with stainless steel;

- Welding of high-temperature alloys;

- Welding high carbon steels, etc.

These welds were subjected to the following tests and investigation:

- 2D and 3D computed tomography;

- Metallographic investigation;

- Mechanical tests (impact Sharpy test, tensile test, three point bend test, microhardness);

- Chemical analysis;

- Fractography.

The report will be presented to all the results of this work.

Lamberti Carlo
Professor
Scientific Director

Understanding the SCR mechanism in Cu-SSZ-13 catalyst with in situ and operando XAS and XES techniques

SCIENTIFIC ORGANIZATION

Southern Federal University

ABSTRACT

Cu-SSZ-13 is a highly active catalyst for the NH3-assisted selective catalytic reduction (SCR) of the harmful nitrogen oxides (NOx, x=1, 2). Herein, we combined XAS and XES spectroscopies, complemented by FTIR and EPR, with DFT computational analysis to elucidate the nature and location of the most abundant Cu-sites upon different reaction-relevant conditions and on this basis suggest a consistent mechanism for the NH3-SCR reaction.

KEYWORDS

Zeolites, XAS, XES, EXAFS, XANES, FTIR, DFT.

ACKNOWLEDGEMENTS

Authors acknowledge Mega-Grant of Ministry of Education and Science of the Russian Federation (14.Y26.31.0001) for funding the research.

SUMMARY

Cu-SSZ-13 is a highly active catalyst for the NH3-assisted selective catalytic reduction (SCR) of the harmful nitrogen oxides (NO_x, x=1, 2). Since the catalytically active sites for this reaction are mainly represented by isolated Cu ions incorporated into the zeolitic framework, the element-selective study of Cu local environment is crucial for understanding of the enhanced catalytic properties of this material. Herein, we combined XAS and XES spectroscopies, complemented by FTIR and EPR, with DFT computational analysis to elucidate the nature and location of the most abundant Cu-sites upon different reaction-relevant conditions and on this basis suggest a consistent mechanism for the NH_3-SCR reaction.

Langdon Terence
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Recent developments in the processing and properties of ultrafine-grained materials

SCIENTIFIC ORGANIZATION

University of Southampton

ABSTRACT

Ultrafine-grained (UFG) materials have grain sizes within the submicrometer or nanometer range and they are prepared through the application of severe plastic deformation using processing techniques such as equal-channel angular pressing or high-pressure torsion. This report describes recent developments in interpreting the properties of these UFG materials including evaluating the paradox of high strength and low ductility and examining the potential for developing a weakening effect in some materials.

KEYWORDS

Nanostructured materials; Severe plastic deformation; Ultrafine-grained materials.

ACKNOWLEDGEMENTS

This research was supported by the European Research Council under ERC grant agreement no. 267464-SPDMETALS.

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Junior scientist

Advanced synchrotron techniques for operando characterisation of Cu-CHA deNOx catalyst

SCIENTIFIC ORGANIZATION

Southern Federal University

ABSTRACT

Synchrotron-based spectroscopic techniques, namely XANES, EXAFS and XES, have been applied to shed light on the details of local geometry and electronic structure of catalytically active Cu centers in Cu-exchanged chabazite zeolite under operando conditions. Complemented by extensive theoretical analysis, obtained data provided an insight on the mechanism of the deNOx process catalysed by Cu-CHA zeolite.

KEYWORDS

Catalysis, synchrotron, XANES, EXAFS, XES, operando.

ACKNOWLEDGEMENTS

This work was supported by the Mega-Grant of the Russian Federation Government no. 14.Y26.31.0001. K.A.L. acknowledges support from the Scholarship of the Russian President for young scientists СП-2796.2016.

SUMMARY

The current contribution summarizes our three-year work on Cu-CHA zeolite, which is a very promising material for the selective catalytic reduction of harmful NOx gases from industrial and car exhausts. We have performed several X-ray absorption and X-ray emission experiments at ESRF synchrotron (Grenoble, France) to collect an extensive set of data, allowing to characterize the material in many reaction-relevant states. Particularly, due to the combination of experimental and theoretical work we were able to shed light on the local environment and electronic structure of Cu ions hosted in the cavities of the zeolitic framework after the activation of the material in both inert and oxidative atmospheres, upon interaction with gases of SCR mixture and in operando SCR conditions. This allowed us to develop a consistent mechanism of the SCR reaction and to prove its main stages.

Lotarev Sergey

PhD in chemistry

Senior researcher

Direct laser writing of waveguiding crystalline channels in lanthanum borogermanate glasses

SCIENTIFIC ORGANIZATION

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ABSTRACT

Femtosecond laser-induced crystallization of lanthanum borogermanate glasses with chemical composition around stoichiometry of the ferroelectric LaBGeO5 phase has been studied. Applying a focused beam with elliptical cross-section of the waist is shown to improve homogeneity of the laser-written LaBGeO5 crystalline channels. An efficient technique of seed crystal growth using a beam with gradually increasing pulse energy which stabilizes and reduces time required to grow a seed is suggested.

KEYWORDS

Direct laser writing, space-selective crystallization, femtosecond laser, lanthanum borogermanate glass, LaBGeO5.

ACKNOWLEDGEMENTS

The work was financially supported by Ministry of Education and Science of Russia (grant 14.Z50.31.0009) and Russian Foundation of Basic Research (grants 14-03-00931, 16-03-00541 and 16-33-01050).

SUMMARY

Femtosecond laser direct writing of crystalline channels possessing waveguide properties in glasses gives an opportunity to combine functionality of crystals (e.g. luminescent or nonlinear optical properties) and flexibility, manufacturability and low cost of oxide glasses. This technique based on high repetition rate femtosecond regenerative amplifiers (typically 250 kHz) developed during the latest decade is now regarded as a promising way for active components of integrated optical devices [1-3]. Formation of quasi single-crystalline channels typically consists of two steps including initiation of a seed microcrystal inside the glass by the tightly focused stationary femtosecond laser beam and growth of a crystalline channel from the obtained seed by moving the waist of the laser beam along the predetermined path with a constant speed. Best results have been so far obtained in $25La_2O_3{\cdot}25B_2O_3{\cdot}50GeO_2$ glass in which femtosecond laser-written multimode waveguiding channels consisting of the ferroelectric stillwellite-like $LaBGeO_5$ phase and showing optical losses of about 2.5-3 dB/cm were reported [3]. Recently, we have demonstrated that femtosecond laser-induced growth of oriented crystalline channels in this glass can be realized at much smaller pulse repetition rate starting from ~25 kHz [4].

In the present study, femtosecond laser-induced crystallization of lanthanum borogermanate glasses with chemical composition around stoichiometry of the ferroelectric $LaBGeO_5$ phase has been investigated using a femtosecond ytterbium laser TETA (wavelength 1030 nm, pulse duration 290 fs, pulse energy up to 0.11 mJ, pulse repetition rate up to 100 kHz).

A technique of seed crystal growth using a beam with gradually increasing pulse energy is suggested. It stabilizes and reduces time required to grow a seed crystal and allows obtaining it in glasses with lower crystallization ability as compared to the beam with a constant pulse energy. This technique also allowed us crystallization of glasses with a chemical composition shifted from the stoichiometric composition of the precipitating $LaBGeO_5$ phase. It has been demonstrated that lower crystallization ability of these glasses as compared to $25La_2O_3{\cdot}25B_2O_3{\cdot}50GeO_2$ glass enables growth of more homogeneous crystalline channels presumably due to lower concentration of undesirable crystallites on the way of the growing channel but at the same time drastically hinders precipitation of the seed crystal with a conventional beam with a constant pulse energy. Thus the glasses with shifted composition could be crystallized only using a beam with an increasing pulse energy.

Another enhancement of the earlier experimental technique has been applying a focused femtosecond beam with elliptical cross-section of the waist aligned along the writing direction enabled further improvement of the homogeneity of the laser-written $LaBGeO_5$ crystalline channels.

As a result, crystalline channels obtained in the bulk of $25La_2O_3$-$30B_2O_3$-$45GeO_2$ glass noticeably deviating from the chemical composition of the crystal showed a waveguide effect and optical losses measured at 1030 nm were not higher than 1.6 dB/cm which is somewhat less that was reported earlier for the analogous channels in $25La_2O_3{\cdot}25B_2O_3{\cdot}50GeO_2$ glass [3].

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ADDITIONAL INFORMATION

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Director

Innovative materials based on thermoplastic polymers

SCIENTIFIC ORGANIZATION

Institute of Macromolecular Compounds Russian Academy of Sciences

ABSTRACT

Modern composite materials based on thermoplastic polymers possess unique set of properties and could be used as a replacement for traditional construction materials in automotive, aerospace and shipbuilding industry. Development of such material requires deep understanding of relationship between their structure and properties. Multiscale computer simulation accompanied by experimental studies is one of the most advanced methods to study such materials, and predict their properties.

KEYWORDS

Multiscale computer simulation, composite materials, molecular dynamics, thermoplastic polymers.

ACKNOWLEDGEMENTS

This study was supported by the Russian Ministry of Education and Science within the State Contract No. 14.Z50.31.0002 (Megagrant). The simulations were performed using the computational resources of the Institute of Macromolecular Compounds, Russian Academy of Sciences, and the Chebyshev and Lomonosov supercomputers at Moscow State University.

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In vivo Visualization of Nanocomposite Microcapsules Addressed by Magnetic Field Gradient

SCIENTIFIC ORGANIZATION

Saratov State University

ABSTRACT

Microcapsules have a number of advantages, such as high loading efficiency, possibility to add magnetic nanoparticles and fluorescent substances into a capsule that allows to track and control of microcapsules in vivo. We describe using composite microcapsules for research its remote control in vivo by magnetic field gradient. The visualization of microcapsules in vivo was underway by Near-Infrared Fluorescence Imaging for Real-Time. This approach opens up new possibilities for targeted delivery of drugs.

KEYWORDS

Microcapsules, in vivo, magnetic field, near-infrared fluorescence imaging.

ACKNOWLEDGEMENTS

The work was supported by Government of the Russian Federation (grant №14. Z50.31.0004 to support scientific research projects implemented under the supervision of leading scientists at Russian institutions and Russian institutions of higher education) and Ministry of Education and Science of Russian Federation (project № 2952).

SUMMARY

One of the fast developing directions of research in the nanomedicine area is optical imaging in vivo. The common method of visualization enables carry out bioluminescent and fluorescent imaging for biological processes. This is method used for looking at biodistribution by significantly amount reducing of required animals and increasing of experimental data for each animals in interest region. Polyelectrolyte microcapsules have interest as potential containers for drug delivery due to ease of preparation, multifunctionality and sensitivity to external influence. Microcapsules have a number advantages, such as high loading efficiency, possibility for load a magnetic nanoparticles and fluorescent substances into a capsule which allows to track and control of microcapsules in vivo. We described to using composite microcapsules for research a distant control in vivo by magnetic field gradient. The visualization of microcapsules in vivo was on stage by Near-Infrared Fluorescence Imaging for Real-Time. The microcapsules contain magnetite nanoparticles (FeNP) and fluorescent dye – Cyanine 7 NSH-ester conjugating with bovine serum albumin (BSA-Cy7) and polyarginine (pArg). The average size of microcapsule was about 5±1μm and 0.7±0.1μm. The microcapsule suspension injections into tail vein (systemic administration) and into femoral artery (local administration) were proposed out respectively. The magnetic targeting of microcapsules with average size 0.7±0.1μm for femoral artery injection is more efficient compare with tail significantly higher comparison tail vein injection was established. This approach open new possibilities for targeted drugs delivery system.

Michailov Vesselin
Professor

Lightweight materials and structures – today and tomorrow

SCIENTIFIC ORGANIZATION

Brandenburg Technical University Cottbus-Senftenberg

ABSTRACT

The engineers have already reduced the structure weight with application of materials with low density and high strength. One important way for weight reduction is also the increasing of the stiffness of the construction by structured or layered materials. The present work describes the motivation of lightweight materials and structures developing as well as their modern processing technologies, e.g. Short Arc Welding and Friction Stir Welding. A new Impulse Friction Stir Welding Method is presented and its influence on the strength of the welded joints is discussed.

KEYWORDS

Lightweight materials and structures, Industrial applications, Aluminium Foam Sandwiches, Impulse Friction Stir Welding, Numerical FE-Simulation, Mechanical Properties.

ACKNOWLEDGEMENTS

The research has been performed at Peter the Great St. Petersburg Polytechnic University under the contract № 14.Z50.31.0018 with the Ministry of Education and Science of the Russian Federation.

SUMMARY

The present work gives fundamental overview about the modern lightweight materials and their applications for reliable structures like aircrafts, vehicles and trains. Almost all innovative products are also characterized by energy efficiency and sustainability of structures. In nearest future a lot of composites with carbon fibers and different laminates will be used in production scale. Lightweight materials such as aluminum and magnesium based composites will have a huge potential for the future development.

Another trend to reduce the weight of the structure is the increasing of stiffness by structured sheets, extruded Al-Panels or Al-Foam-Sandwiches (AFS). In the last one Al offers not only its low density and the good mechanical properties but also the advantage that it is extremely suitable for foaming due to the relatively low melting point. Furthermore, it offers the particular possibility of manufacturing a strong, large-area material joint-AFS, due to the utilisation of a similar material combination – conventional or structured sheets in the cover layers and aluminium foam in the core. The semi-finished AFS products can be processed flexibly in the still unfoamed condition as well as in the already finish-foamed condition. Investigations into the welding and the resulting joint properties are necessary so that the advantages of AFS can be used effectively as a material for welded structures. In the presented paper, systematic investigations were conducted into the weldability of AFS in the foamed and unfoamed conditions, mechanical-technological properties of the joints (joining nodes) were established and FEM modelling procedures were carried out.

The problem of joining for such type of similar and especially dissimilar materials can be solved preferably by means of Friction Stir Welding (FSW). The FSW developing to Impulse Friction Stir Welding (IFSW) and the influence of impulse parameter on the mechanical properties of the welded joints are discussed in the third part of the presentation.

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PhD of Physico-Mathematical Sciences

Research fellow

Laser nanoengineering of biocompatible scaffolds and microbial systems

SCIENTIFIC ORGANIZATION

Institute of Photonic Technology of Federal State Establishment «Federal Research Center «Crystallography and photonics» RAS

ABSTRACT

Have been created system of femtosecond laser microstereolithography to form the structures of polymer composite materials. Has been developed a technique of formation of bioresorbable scaffolds with a complex structure for engineering of soft and hard biological tissue. Have been created systems for of realization of the method of laser microsampling. Have been developed method that allows using short laser pulses to separate individual microbial cells together with their surroundings area from the substrate plate and transfer them to the culture medium for further cultivation.

KEYWORDS

Laser stereolithography, two-photon polymerization, laser printing, laser microsampling.

ACKNOWLEDGEMENTS

Head of megaproject Chichkov Boris Nikolayevich. Employees of the Institute of Photonic Technology FSI FNITS “Crystallography and photonics” RAS: Bagratashvili Viktor Nikolaevich, Timashev Peter Sergeevich, Bardakova Ksenia Nikolaevna, Koroleva Anastasia Valerievna, Pudovkin Galina Ilinishna, Chutko Yekaterina Aleksandrovna, Churbanova Yekaterina Sergeyevna and other colleagues. Employees of the Faculty of Soil Science: Kachesovu Kirill Igorevich, Gorlenko Mikhail Vladimirovich, Lysak Lyudmila Vyacheslavovna.

SUMMARY

Currently, the use of laser technology for three-dimensional bio-printing or manipulation of biological objects is one of the most important trends in modern science. Laser radiation allows highly effective dosed local impact with high performance on the required objects. The reliability of modern equipment allows to carry out the necessary process around the clock for a long time. This work is aimed at the development of this technology and methods for the subsequent implementation of the results in the field of regenerative medicine and pharmacy.

Part 1. Formation biocompatible scaffolds by two-photon femtosecond micro stereolithography.

Technology for creating biocompatible tissue-engineering structures using three-dimensional printing method is currently experiencing exponential growth. Early experiments in this direction have shown in practice possible to obtain fragments of different tissues and organs. The decisive step in the development of organ recovery technology is the ability to create a biocompatible porous matrix - “scaffolds”. Scaffolds for tissue engineering be used as a temporary substrate for attachment and growth of cells and must correspond a lot of requirements, such as biocompatibility, bioresorbable, compliance with specified mechanical properties.

One of the most of perspective methods for solving this problems is two-photon femtosecond photopolymerization. This method allows to carry out with high efficiency process of radical polymerization of micron size area to filling a volume of scaffold for by three-dimensional model using the femtosecond laser. We used the photo sensitivities compositions based on chitosan and its copolymers with photoinitiator Irgacure 2959 (Ciba ®), and with the addition of various crosslinkers and photo sensitivity polylactides materials.

The complex of two-photon femtosecond laser micro-stereolithography (Fig. 1) has been created within the work. We used second harmonic laser «TeMa-100» (Avesta-Project, Russia) (Fig. 1a) as a femtosecond light source. Laser radiation was controlled by acousto-optical modulator (Fig. 1b) on frequencies up to 1 MHz. To adjust the output power used optical system (Fig. 1c), consisting of a half-wave plate, a polarizing beam-splitting cube and power meter. As a focusing element used microscopic planar lenses, mounted on galvoscanner (Fig. 1e), which provides

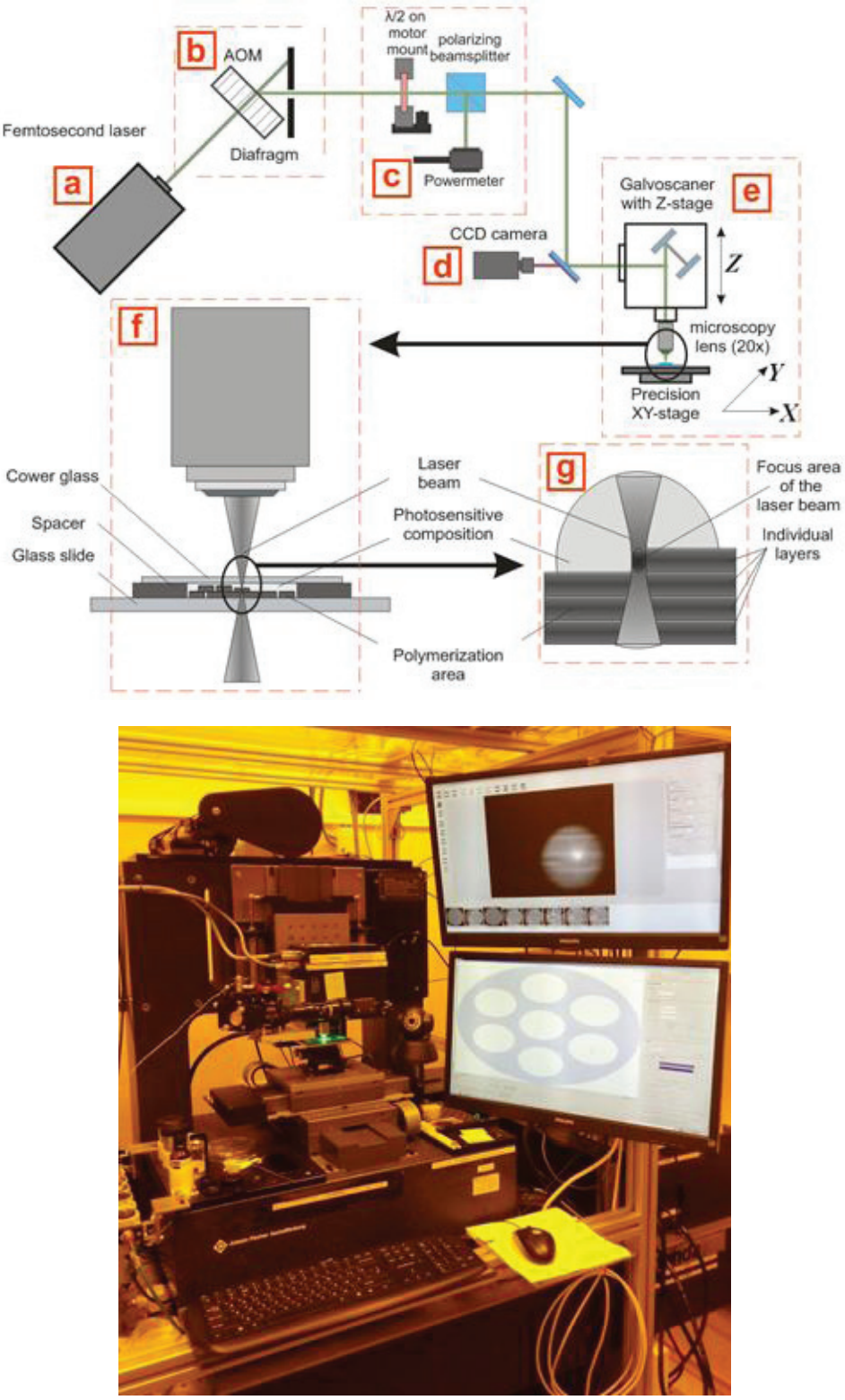


Fig.1 Photo and a schematic of the two-photon laser micro-stereolithography.

high-speed movement of the focused laser beam in the focal plane of the microscope objective. Galvoscanner is mounted on the Z-precision of three-axis table motions ABL-1000 (Aerotech, USA), which provides a change of the laser focus in the required plane using a CCD camera with a objective (Fig. 1d). The submicron positioning accuracy of the system was provided by the movement of the table along the rails on an air bearing using linear brushless servomotor, feedback presence, controlling the position with an accuracy of nanometers and a massive granite base, mounted on viboisolated optical table. A photosensitive composition was placed on a glass slide, was limited to a silicone spacer and a cover glass (Fig. 1f), through which the laser light delivered by a given program in accordance with computer model.

In the center of the focused laser light is a region with the shape of ellipsoid prolate in the vertical axis. Inside this region by the influence of high-intensity femtosecond laser pulses took place two-photon absorption, causing the collapse of the photoinitiator into radicals that trigger the process of three-dimensional cross-linking (Fig. 1g). Depending on the used microscope lens height crosslinkable region was 1-8 μm, and the diameter of the cross section along the XY axes was 0.3-4μm. Area size also depends on the size of the laser power. Filling volume polymerized structure was made in layers-by-layers. With the help of galvoscanner laser beam filled area of each layer separate lines for a program at a high speed. Then, the focus shifted in the vertical plane through the axis Z-translator and start irradiated next layer. Thus, the whole volume of three-dimensional model was filled by creating unit volumes of the structures of the polymerized composition inside the starting material. Then, with the X-Y translator sample shifted to a new location and repeat the process a single structure polymerization. According to the described method create an array of contiguous structures polymerized unit predetermined configuration, providing quick filling of the entire volume scaffold with micron or submicron resolution and high productivity.

In the first stage, as unitary structures used model of a hollow cylinder with an outer diameter equal to the diameter of the microscopic field 20x lens - 250 mm (Fig.

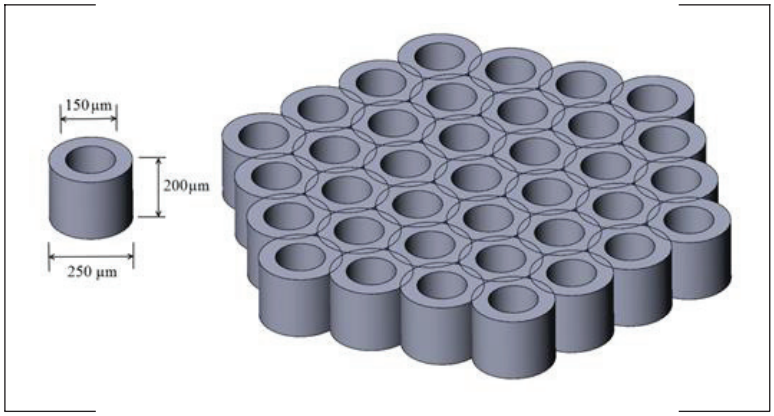


Fig.2 Image of unit structure (left) and model of scaffold (right).

2). Structure printed in a hexagonal order with little overlap with each other, forming a periodic porous scaffold.

To increase the productivity of manufacturing scaffolds, as a single unit structures was decided to use a microscopic lens with a smaller increase, but with a larger diameter of the field (400mkm). It is possible to use more complex unit structure (Fig. 3), Through which matrixes formed for model experiments on prototypes tsitosovmestimost materials and scaffolds for the cultivation of neuronal cells.

Currently, work is underway to create scaffolds from other unit models with a complex structure that allows, controllable place different cell cul-

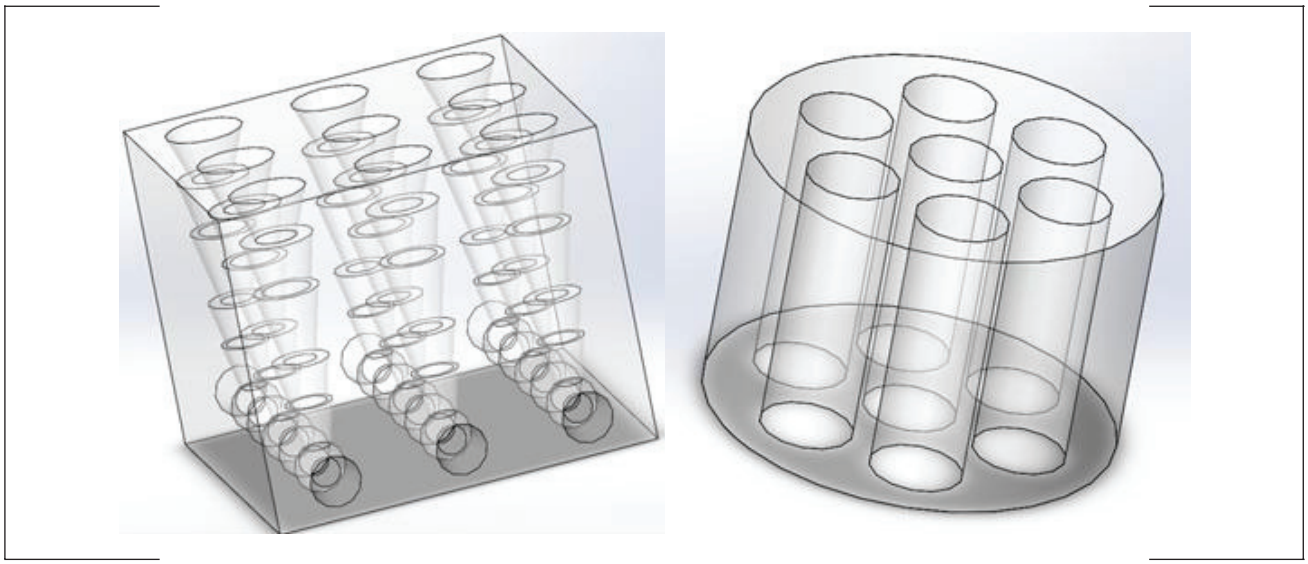


Fig.3 Image of unit structures used for experiments on cytocompatibility scaffolds (left) and model used for the cultivation of neural scaffolds for preclinical testing (right).

tures in the internal volume the scaffold. Work is under the selection of the optimal parameters of scaffolds, for example for different cell cultures - mesenchymal stem cell or neuronal cells. The results of this work will be presented at the conference.

Part 2. Application of laser bioprintinga for manipulating microbiological objects.

Two years ago, a group of scientists (Ringeisen et al, 2014) demonstrated the possibility of cultivation of microorganisms in the soil microportions isolated using laser radiation. To do this, they used a method based on laser bioprinting (Laser-assisted bioprinting, LAB). In laser bioprintinge biomolecules and living cells are mixed with a hydrogel and applied on a glass plate with a laser radiation absorbing thin metal layer. This substrate is called the donor, inverted and subjected to laser irradiation. A laser pulse is absorbed in the metal layer, the metal evaporates and between the glass plate and hydrogel the steam bubble is formed. The expansion and subsequent collapse of the bubble leads to the formation of a hydrogel spray. Thus, each laser pulse results in the transfer of the printed droplets with a donor material to the receiving plate disposed in parallel or in a well of a standard microbiological plate. The above mentioned group of scientists made the transfer of microportions soil with diameter from 170 to 430 micrometers on the glass or in the culture medium, using ultraviolet laser radiation. Due to the nature of the experiment - the transport of dry soil, there was a strong sprinkling of soil, the amount of transferred particles was great, it is not possible to talk about the isolation of individual colonies of microorganisms, and it was not received definitive data on the survival of microorganisms.

In this work we propose a new method of laser transfer of soil particles in a liquid medium. It is applicable to any soil, provides vitality, allows you to transfer a given concentration of the soil particles. It was designed and engineered plant-based fiber laser infrared (NTO “IRE-Polus”, Russia) and galvoscanner with F-theta lens with a working field of 100 * 100mm and motorized XY table for moving the receiving glass plate or a standard microbiological plate.

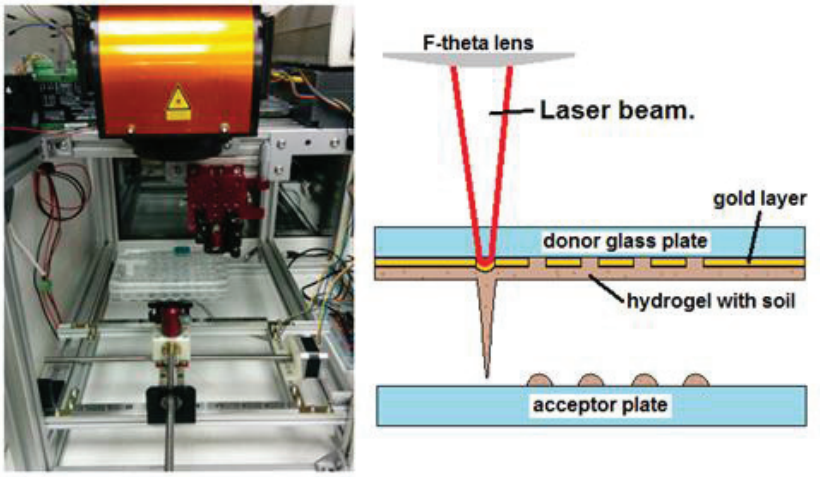


Fig.4 Photography of prototype system with mounted microbiological tablet (left) and scheme of transfer soil particles (right).

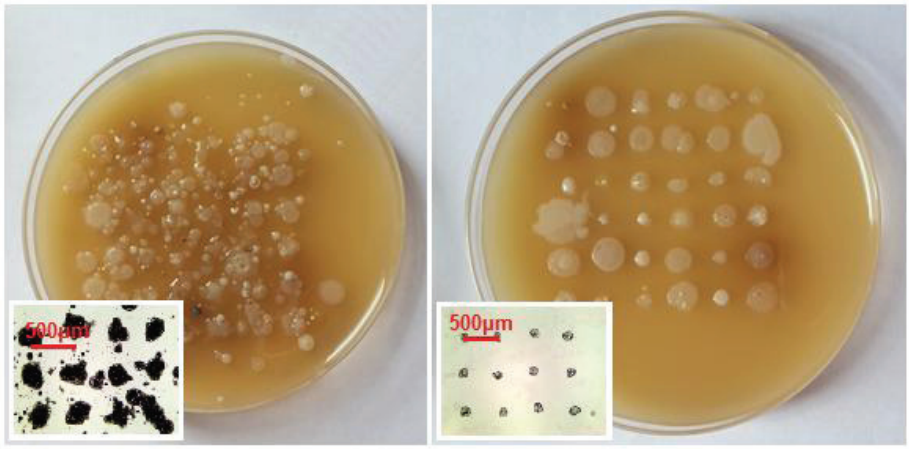


Fig.5 Photo of Petri dishes with the nutrient medium after laser transfer array drops of soil mixture with water (left) and a mixture of water and soil hydrogel (right). Insets show pictures of the results of experiments with the transfer of the soil on a glass plate.

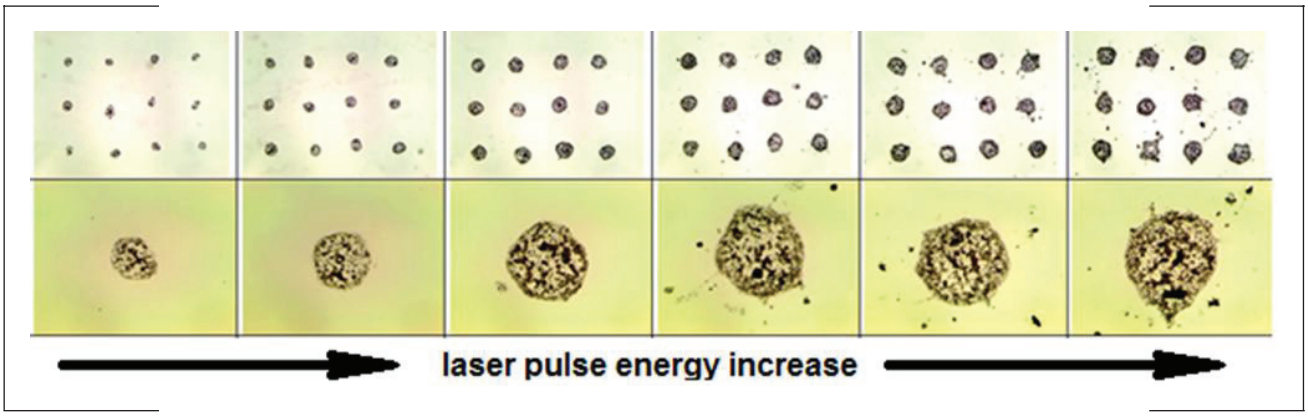


Fig.6 Photo of drops soil mixture with hydrogel after transfer of laser with different energies of the laser radiation.

In this configuration, experimental system allowed to carry out high-speed transfer of small soil particles, operating a laser beam with a spot diameter at the focus ~ 30 μm with adjustable pulse duration (from 4 to 100 ns) and pulse energy (from 10-100 μJ).

Decisive importance in the laser transfer process is the energy of the laser pulse. There is a threshold below which the soil transfer was not observed. With the laser pulse energy increases (Fig. 6), the increase in droplet size observed, as demonstrated through experiments on the receiving plates. Also, an increase leads to disruption of the droplet shape and appearance of the spray, which is associated with an increase in speed of the jet and the violation of its laminar.

A result of experiments were identified modes of laser printing by soil particles with microorganisms in the liquid and solid culture media, optimized modes of laser system with finding the laser energy threshold for effective transfer. The results of analysis of direct sowing data on solid agar growth medium were obtained. Spend

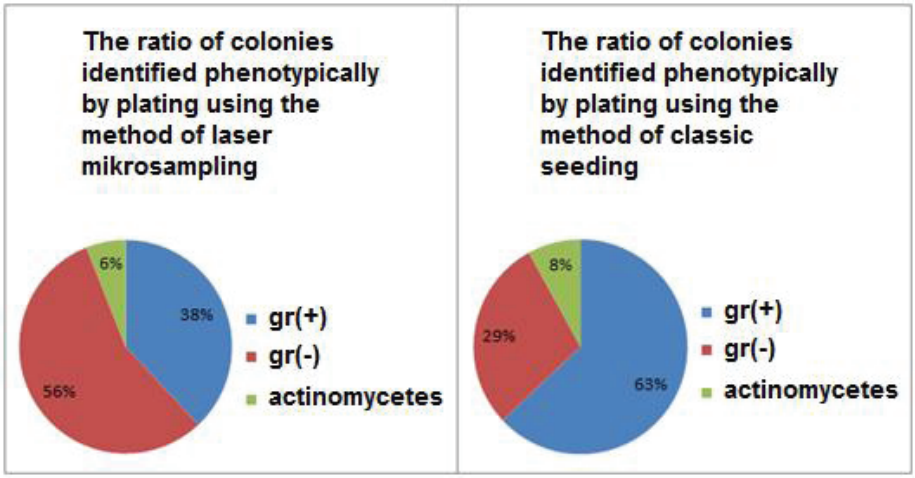
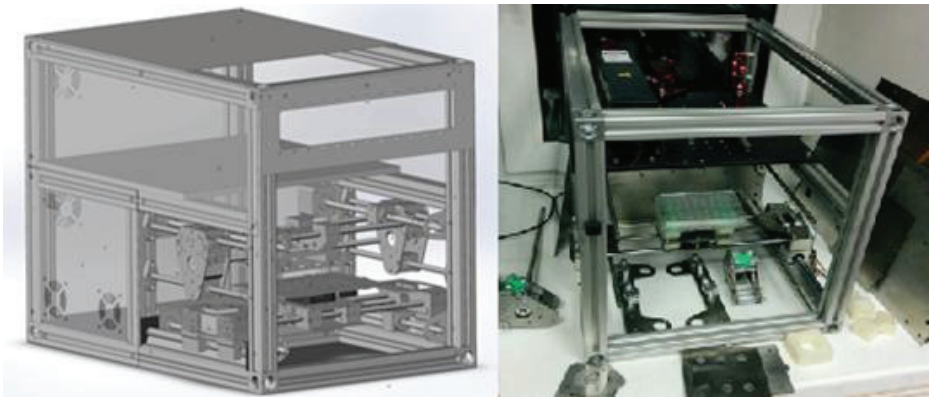


Fig.7 Distribution of the groups of microorganisms in percentage using a laser transfer method (left) and the classical method of seeding (right).

Fig.8 The three-dimensional model of the second prototype of the installation of the laser transfer (left) and install the photo in the process of creating, as of May 2016 (right).



the processing parameters of the structural biodiversity accounted forms. The results of evaluation of the functional biodiversity of microbial objects received via MCT method, show significant differences in the structural and functional characterization of microbial communities chernozem soil due to the impact of laser transfer procedure.

According to an analysis of more than 600 colonies revealed significant differences on the basis of the analysis of phenotypic traits (by direct microscopy) and KOH reaction distributions Gram-positive and Gram-negative organisms to the classical method of planting and seeding and laser transfer of microorganisms (Fig. 7)

At the current moment a new version of the installation, allowing to carry out the process of the transfer of laser to operate in a fully automatic mode. System adapted to work with the 1 or 2 standard microbiological tablets. Installation of the process allows for working at the same time with several substrates with different types of objects supported on different receiving plate or in specified wells microbiological plate. The possibility of of observation through a digital camera with a microobjective on the samples before, during and after exposure. It is possible to select the diameter of the laser beam spot is in the range of tens to hundreds of micrometers, the ability to fine tune the laser power. The design is maximally adapted to operate in a laminar flow hood. As of May 2016 is in the final assembly and adjustment.

Molodtsov Serguei
Prof. Dr.
Scientific Director

European XFEL – novel tool for nanomaterials research and characterization

SCIENTIFIC ORGANIZATION

European XFEL

ABSTRACT

The European X-ray free electron laser (XFEL) is a new international research installation that is currently under construction in the Hamburg area in Germany. The world-unique feature of this free electron laser is the possibility to provide per second up to 27.000 ultra-short (10 - 100 fs), ultra-high brilliance flashes that makes this facility particular suitable for nanomaterials research and characterization. In this presentation, selected examples of experiments will be given and plans for implementation of dedicated instrumentation at the European XFEL will be described.

KEYWORDS

Nanomaterials, megaprojects, ultrahigh time resolution.

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Empirical and theoretical approach to optimize the gas-powder flow in laser additive technology

SCIENTIFIC ORGANIZATION

Kazan National Research Technical University named after A.N. Tupolev

ABSTRACT

This work presents the results of numerical and experimental optimization of gas-powder flow in subsonic and supersonic laser cladding systems. The following subsonic types of cladding heads were investigated: off-axis nozzle, coaxial nozzle, and four-jet nozzle. High-speed imaging and shadow imaging are shown to be effective tool to optimize aerodynamics for both subsonic and supersonic nozzles. Proposed numerical simulation of supersonic gas streams takes into account convective and conductive heat transfer and turbulence.

KEYWORDS

Laser additive technology, laser cladding, schlieren method, gas-powder flow, hight speed visualization.

ACKNOWLEDGEMENTS

The work is supported by the Ministry of Education and Science of the Russian Federation (government contract №14.Z50.31.0023)

SUMMARY

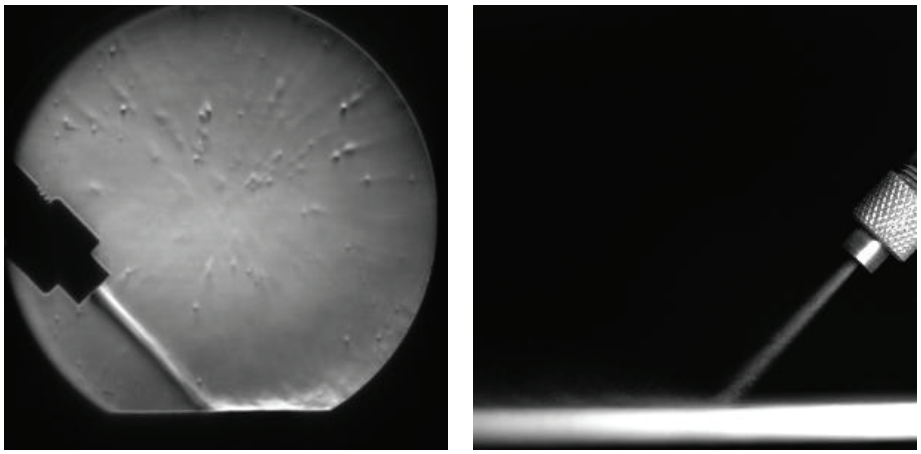
Laser powder cladding is widely used for protective and functional coatings of metal surfaces, recovery of broken shapes, as well as for layer-by-layer additive synthesizing of metal products. Multi-jet nozzles are typically used for powder deposition. These nozzles differ by functionality and mutual orientation of the powder jet and laser beam. Dynamics of protective and transport gas at the nozzle's outlet and in vicinity of the substrate plays an important role in the formation of a powder jet. Supersonic laser cladding is a rapidly developing method of additive laser technology. It combines the advantages of a classical subsonic laser cladding and a cold gas spraying. Gas flow dynamics between the nozzle and the substrate as well as temperature distribution in area of powder coating take a significant effect on cladding quality and metallurgical contact between coating and the substrate.

That is why experimental and numerical study of gas-powder flow dynamics in subsonic and supersonic nozzles for laser powder cladding seem to be relevant.

Visualization of transport gas and shielding gas flow was performed by shadow Schlieren method on original experimental equipment. High-speed imaging with the "laser knife" lighting system and a laser Doppler anemometer are used to study the flow of powder jets. Spatial distribution of temperature on the substrate was measured by means of FLIR SC7700 BB thermal imaging camera. Thermal vision experiments and gas flow visualization were done simultaneously.

Modeling of heated supersonic gas flow leaving de Laval nozzle is based on transient numerical solution of full set of the Navier-Stokes equations using the control volume method with the SIMPLE pressure correction technique (semi-implicit method for pressure-linked equations). In addition, the energy equation and the gas state equation were solved simultaneously. Consequent turbulent effects are simulated using the large eddy simulation model (LES).

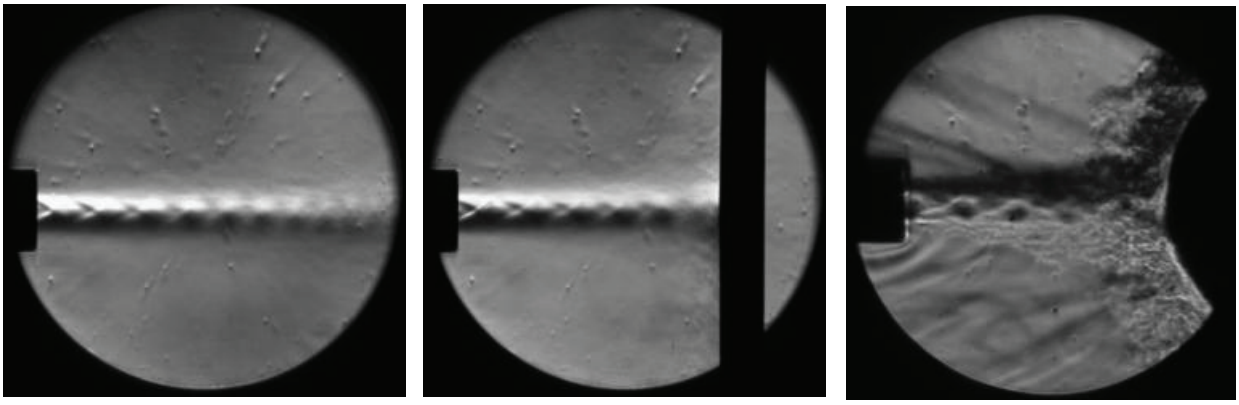
Visualization of gas-powder flow in an off-axis nozzle showed that diameter of orifice in cyclone's cap plays an important role in formation of powder flow. This orifice resets the atmosphere of excessive transport gas. Diameter of each type of nozzle has a corresponding optimal diameter of cyclone's orifice to produce the most stable and focused flow of powder particles.



(a) (b)

Figure 1. Off-axis nozzle for laser cladding:
a - shadow image of the transport gas stream; b - a frame from a high-speed video of the powder particles flow

Spatial structure of supersonic gas flow and transient temperature fields on the substrate in supersonic laser cladding system are investigated via Schlieren shadow imaging and the thermal vision system. Smoothness of inner surface of the de Laval nozzle is crucial for the stability of outer gas flow. Welded powder particles occasionally precipitate inside the nozzle and make the supersonic flow unstable. Heated supersonic gas stream becomes much less stable than the cold one. However, the heating area of the substrate has a symmetrical shape within the diameter of supersonic gas jet. It means that the shape of the gas jet stays constant before the collision with the substrate.



(a) (b) (c)

Figure 2. Shadow image of nitrogen stream for the supersonic nozzle for laser cladding
a - the flow in the free space, the room temperature of the gas;
b - flow with a flat obstacle, room temperature of the gas;
c - flow with a cylindrical obstacle, gas temperature 500 ° C

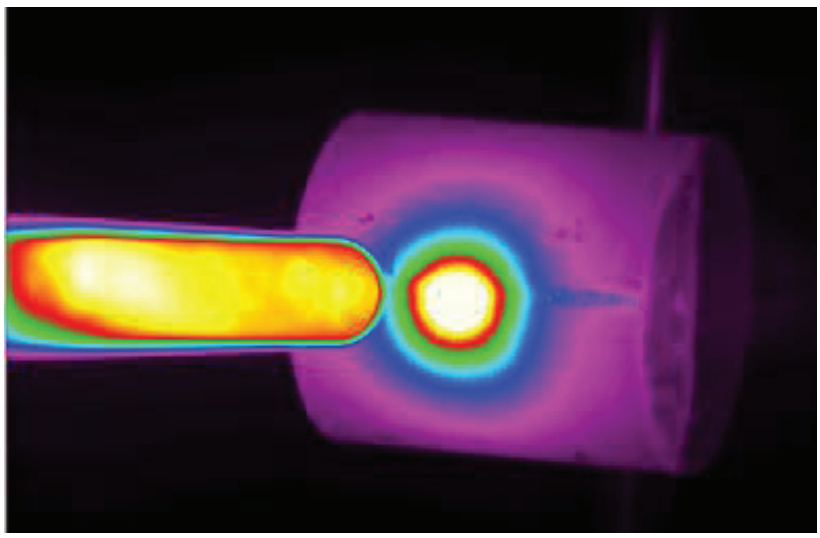


Figure 3. Thermal image of the cylinder treated by supersonic flow. The gas temperature 500 ° C

Numerical experiments revealed that the gas flow at the end of the nozzle has much lower velocities than the ones within the nozzle. This effect is observed in a wide range of boundary conditions on temperature and pressure of the gas entering de Laval nozzle. Average length of the gas jet decreases with temperature according to a quadratic law. This effect has the following explanation: the viscosity of a heated gas is greater than the one for cold gas. The results of the modeling are in good agreement with the data obtained via high speed Schlieren imaging.

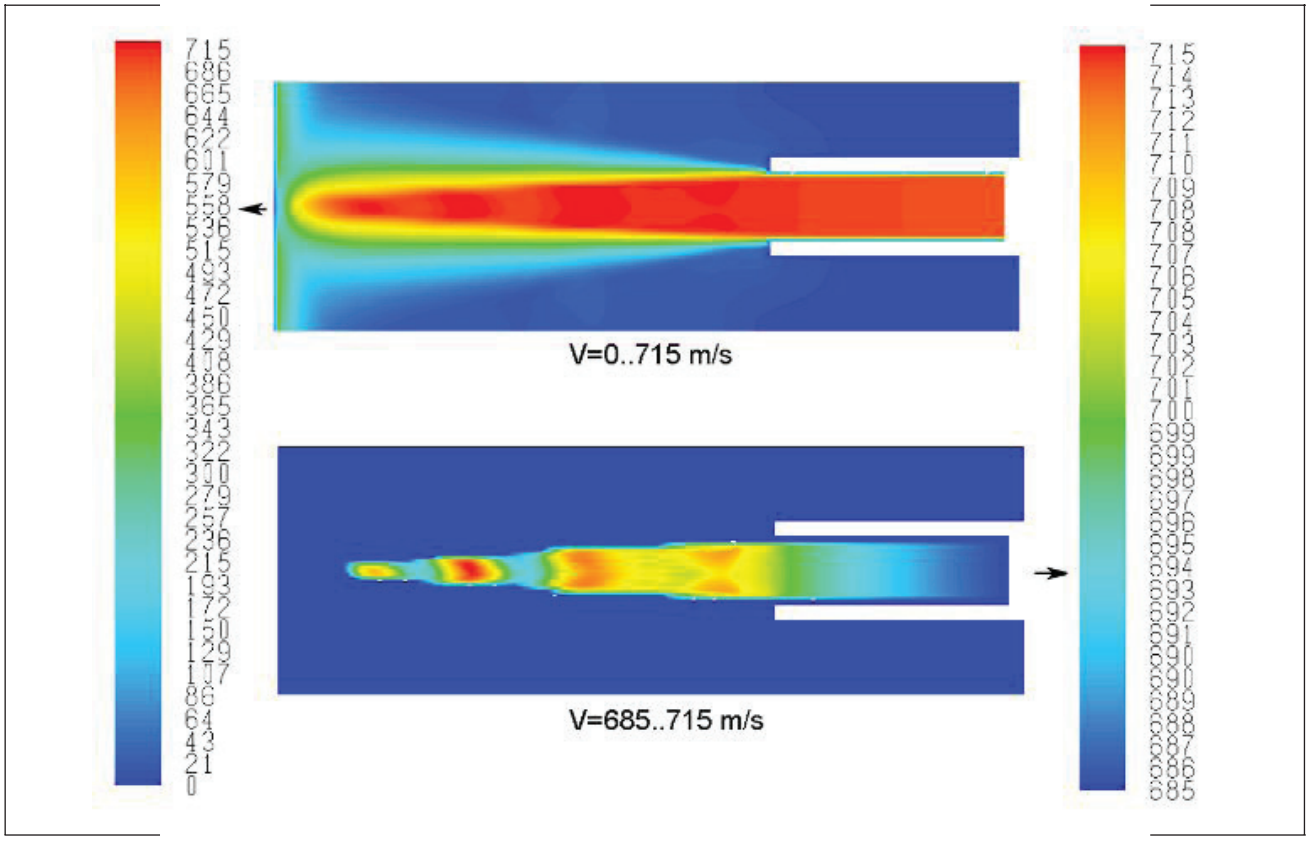


Figure 4. The modeling results. Inner flow pattern: acoustic shockwaves.

Naumov Anton
PhD
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Microstructure formation during friction stir welding of high strength aluminum alloys

SCIENTIFIC ORGANIZATION

Peter the Great St. Petersburg Polytechnic University

ABSTRACT

In the present research the results of Friction Stir Welding of two Al-based alloys with Mg and Cu are presented. The temperature distribution during FSW with the help of thermocouples was measured and was compared with the results of numerical FE-simulation with program ANSYS. Fourteen points of the welds were taken for the detailed analisys of thermocycles and microstructure formation. The thermocycles in these points were simulated on the Gleeble-3800 System, the received microstructures were compared to the microstructures of the points of the welds.

KEYWORDS

Friction Stir Welding, Numerical and Physical Simulation, Microstructure, Gleeble tests.

ACKNOWLEDGEMENTS

The research has been performed at Peter the Great St. Petersburg Polytechnic University under the contract № 14.Z50.31.0018 with the Ministry of Education and Science of the Russian Federation. The authors gratefully acknowledge the support of the President of Russian Federation through the grant № MK-7840.2016.8.

SUMMARY

The Friction Stir Welding (FSW) is the solid state process widely used to provide similar and dissimilar joints. The main advantages of this process are the relatively

low temperatures of welding (0,5-0,8 of the melting point) and the possibility to provide similar and dissimilar joints of materials combinations which are unweldable by conventional methods of welding. The relatively low temperatures of FSW allow to prevent hot cracking and porosity which are typical for conventional welding methods of high-strength aluminium alloys, for example, and to decrease the distortion of welded sheets.

The parameters of FSW for 2 mm butt joints were set for two different materials Al-Mg and Al-Cu alloys to get solid welds. The tool rotation was varied in order to change the temperature of process that has direct influence on the microstructure formation. The number of thermocouples was used during FSW to measure the thermocycles in certain points of the welds. Using this data the numerical FE-model of temperature calculation made in ANSYS was calibrated.

The phanoramic pictures of the welds after FSW were received. The net of 14 points was set for the phanoramic pictures of the microstructure in order to calculate the thermocycles in these points with the help of the calibrated FE-model. The net has 2 rows, the first is 0.5 mm below the upper surface and the second is 0.5 mm over the bottom serface. The analisys of themosycles in upper and lower raws shows the uniform distribution of temperature through the thickness of the 2 mm metal sheets.

The calculated thermocycles were physically simulated using Gleeble-3800 System with Pocket Jaw MCU. The microsructure of received samples was analyzed and compared with microstructure of the points of the welds. The main influence on the microstructure formation has the deformation at the elevated temperatures during FSW.

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PhD student

Spark plasma sintering β-SiAlON-BN ceramic composites

SCIENTIFIC ORGANIZATION

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)

ABSTRACT

Investigated was spark-plasma sintering (SPS) of β-SiAlON-BN (0-30 wt. %) ceramic composites. The base raw materials (β-Si5AlON7 and BN powders) were prepared by infiltration-mediated combustion synthesis (CS). Experimentally established were condition for SPS ceramic composites with high relative density (more than 95 %) and flexural strength 250-300 MPa: (a) heating rates 50 °C/min, (b) maximal temperature 1650–1750 °C, (c) and holding time 5 min.

KEYWORDS

Sialon, boron nitride, ceramic composites, spark plasma sintering, mechanical behavior.

ACKNOWLEDGEMENTS

This work was financially supported by the Russian Foundation for Basic Research (project no. 15-03-01051_a) and the Russian Science Foundation (project no.16-19-10213). The support of the Ministry of Science and Education of Russian Federation (grant 11.G34.31.0051) is gratefully appreciated.

SUMMARY

β-SiAlON-BN ceramic composites - promising materials that can be used in conditions of high mechanical stress, thermal shock, abrasion and exposure to aggressive chemical agents. β-SiAlON-BN composites are highly promising for metallurgical applications such as tubes for metal pouring, pipe heaters, nozzles, dozer units, annular breakers, buckets, crucibles, lining plates, thermocouple casing, sensor level gages, etc.

Among methods for producing powder sialon based materials combustion synthesis (CS) has attracted increasing interest due to the possibility of obtaining products of

high purity in a short reaction time. The most rapid and effective sintering method of ceramic powders, as well as other solid materials, is spark-plasma sintering (SPS). Thus, using a combination of these methods is possible to obtain high-density ceramics composition with improved physical mechanical properties.

Synthesis of initial materials for sintering was based on infiltration-mediated combustion powder mixture of Si, Al and B in nitrogen gas under pressure of 10 MPa. CSed β-Si_5AlON_7 and h-BN powders, were prepared by a high-energy planetary steel ball mill. The milled powders, which weighed about 0.5 g, were placed into a graphite die of 10,4 mm inner diameter and were sintered using a spark plasma sintering system Labox 625 under vacuum condition of lower than 10 Pa. The heating rate was 50 °C/min. The sintered compacts were heated from room temperature to 600 °C without load and were then heated to the desired temperatures (1550-1800 °C) at compressive stress of 50 MPa. The compacts were maintained at the desired temperature for 5 min before the power was turned off. Temperature monitoring during sintering between 600 C and the final sintering temperature was carried out using an optical pyrometer, focused on a hole on the surface of the carbon die.

The particle size distributions of the milled powders were determined via laser scattering method by using Fritsch Analysette 22. The used powders and sintered compacts were characterized by XRD (DRON-3.0) and SEM (JEOL 6610L). Sample densities were determined by hydrostatic weighing. Flexural strength (f) were measured by using universal testing machine (Instron-5966).

As a result, β-SiAlON-BN samples having a relative density of 95-98% were obtained by SPS while sintering pure β-SiAlON powders without additives allows to obtain a density of 85-90% of the samples. Using Y_2O_3 intensified sintering of pure β-SiAlON powder and practically no effect on the shrinkage kinetic compositions of samples β-SiAlON-BN. Introduction Y_2O_3 considerably increases the sintering intensity of β-Si_5AlON_7 at temperatures above 1400 °C, i.e. after formation of the eutectic with liquid oxide compounds. Introduction of h-BN also contributes to obtaining a more dense materials at the SPS, but the mechanism of action of this compound is different. h-BN improves compactibility of sintered powder mixtures. When 30 wt. % content of particles of non-wettable oxide melts, h-BN particles are almost completely isolated of β-Si_5AlON_7 particles from each other. Thus, the relative density of β-SiAlON-BN close to the theoretical value can be achieved without the introduction of Y_2O_3 activator.

The level of the relative density is a determining parameter for the strength characteristics of sintered ceramic composites. Flexural strength ceramic composition samples β-SiAlON-BN increased as compared with the samples obtained under the same conditions but without BN. Deterioration of the mechanical characteristics was observed with BN content increases above 10 wt. %. It is also found that the change in the strength properties of the sintered samples relative to their similar densities dependencies identified earlier in other published works, in the ceramics of similar composition and at least not inferior to them by the value of the magnitude of attainable strength.

Thus, in this work, high-density β-SiAlON–BN (0-30 wt. %) ceramic composites with improved strength properties are obtained at the SPS from CSed raw powders (β-Si_5AlON_7 and BN). Such obtained machinable ceramics seem promising for fabrication of items operating in severe conditions of strong thermal shock and corrosion-active medium.

Additional information

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SCIENTIFIC ORGANIZATION

Stankin Moscow State Technological University

Graphene oxide doped YTZP nanocomposites obtained by spark plasma sintering

ABSTRACT

The use of graphene as a component for developing electroconductive ceramic is being profusely studied. It is a very promising additive as it has excellent mechanical properties, high electrical and thermal conductivities, it is lightweight and its aspect ratio allows reaching percolation with low contents. In this work, 3Y-TZP/G composites were prepared by SPS of Zirconia-GO mixtures. Graphene content as low as 0,29 vol% allows obtaining nanostructured black zirconia but it has to be increased up to 1 vol% in order to reach electrical resistivity <100Ωcm, as it is required for EDM.

KEYWORDS

Zirconia composites, graphene, Spark Plasma sintering, black zirconia.

ACKNOWLEDGEMENTS

Authors would like to thank The Ministry of Education of the Russian Federation supported this work by contract №14.577.21.0089, unique identifier of contract RFMEFI57714X0089.

SUMMARY

Introduction

Yttria stabilized zirconia is widely used as structural material in machinery due to its superior properties, such as high strength, high hardness, and high toughness (1-3). After sintering in oxidizing conditions pure dense zirconia has white colour. Therefore many studies have been performed up today for diversification of zirconia colour (4-9). In this regard the black colour has attracted many research works due to a large panoply of possible high added value applications, i.e. artificial jewellery, luxury watches as Apple Watch for example, knifes, bearing balls, optical devices, inductive charging system, fibre optics components, small precision tools, nozzles or PVD targets. Most of the black zirconia commercial products are fabricated by adding 2 to 10 wt% black pigments as $CoFe_2O_4$ spinel to the starting 3YTZP tetragonal submicrometer powder and subsequent sintering in the temperature interval ranging from $1400^{O}C$ to $1600^{O}C$.

In many of the above mentioned applications, the presence of metals like Co, Fe, is not appropriate due to technical requirements, i.e. PVD targets, inductive charging system, or health problem as allergy to Co, etc. Additionally these commercial materials are not electrical conductors and this is a handicap when facing machining of complex shapes as EDM can't be used for this purpose.

On the other hand, zirconia has a very low thermal conductivity (10-11). This fact has as a consequence a limitation in the dimension of the components to be fabricated by conventional processing routes. Advanced sintering technologies as HP also have limitations concerning the maximum thickness of the samples to be pressed, as heat has to be transferred from the mould to the sample. Spark plasma sintering has also limitations due to the high heating rates used during sintering and as a consequence important temperature gradients take place along the sample. In fact SPS open a new possibility for electric conductive materials as additionally to the heating process by the mould, conductive powders can be heated up by Joule effect during sintering (12-14). As a consequence, SPS seems to be only useful for the case of conductive materials and the most part of ceramics cannot take profit of the advantages of this interesting sintering technology.

The use of carbon nanostructures such as carbon nanotubes (CNTs) and carbon nanofibers (CNFs) as additives for preparing electroconductive ceramics has been profusely studied. Nevertheless, the difficulty for getting good dispersions of CNTs and CNFs in ceramic matrices has limited the progress in this research line. Since the discovery of graphene, efforts have been focused on the use of this carbon nanostructure as reinforcement phase in ceramic matrices. In this sense, graphene

oxide has several key advantages versus graphene regarding its processing such as, i) it can be obtained through a low cost method in high quantities (Kg.), ii) as any oxide it can be homogeneously dispersed in water, and consequently iii) mixtures of any ceramic oxide and graphene oxide can be processed following conventional ceramic's processing routes. On the top of this with a small volume fraction of graphene it is possible to reach the percolation threshold in the bulk sample to become a conductor material.

In the present work we fabricate theoretical dense electroconductive free of pores black zirconia compacts by adding a small fraction of graphene oxide. The obtained compacts were characterized mechanically and electrically. This new functionality (electrical-thermal conductivity) allows the possibility to use SPS avoiding the limitations derived from the low thermal conductivity of zirconia and also allows the machining of complex shaped components by electro discharge machining methods (EDM). The wear of the different composites has been also studied and compared to the behaviour of zirconia alone.

EXPERIMENTAL

Preparation of mixed powders

The starting materials used in this work were ZrO_2 (3YTZP, Tosoh Corp., Japan) with average particle size of 180 nm and Graphene oxide synthesized from synthetic graphite by the modified Hummers method (23). Briefly, this method employs Hummers reagents with small amounts of NaNO3 and KMnO4. Concentrated H_2SO_4 was added to a mixture of synthetic graphite and $NaNO_3$, and the mixture was cooled down using an ice bath. Afterwards, $KMnO_4$ was slowly introduced in small doses to keep the reaction temperature below 20°C. The solution was heated to 35 °C and stirred for 3 h. At that point, a hydrogen peroxide (H_2O_2) 3% solution was slowly poured, giving rise to a pronounced exothermal effect up to 98 °C. The reaction mixture was stirred for 30 min and centrifuged (3700 rpm for 30 min) to discard the supernatant. The remaining solid material was then washed with water and centrifuged again; this process being repeated until the pH was neutral. A colloidal suspension of individual graphene oxide sheets in purified water (1 mg·mL^{-1}) was prepared in 1 L batches and kept under ultrasound for 10 h. Afterwards, the suspension was centrifuged (3700 rpm for 30 min) to discard the filtered supernatant.

A colloidal method was used to prepare the GO/3YTZP powders. 40g of 3YTZP were added into 100 mL of water where the pH was previously fixed to 10 by adding NH4 OH. The 3YTZP powder was dispersed under stirring conditions for 30 min. Then, suspension of graphene oxide was dropwise added in order to prepare the desired composition. Mixed powders were kept stirred for 1h. Then, suspension was dried in a Lab Spray drier (Nano Spray Dryer B-90 Advanced, Buchi) at 110°C exit temperature. The obtained powders were ready to press mixtures.

SPS sintering and characterization

The powder samples were placed into a graphite die with an inner diameter of 20 mm and cold uniaxially pressed at 20 MPa. Then, they were introduced in an SPS apparatus KCE-FCT-H-HP-D25-SD (FCT Systeme, Rauenstein, Germany) under low vacuum (10^{-1} mbar) and sintered at 1400°C for 1 min under an applied pressure of 80MPa and a heating rate of 100°C/min. Bulk density of the sintered bodies was measured by the Archimed's method using water as solvent.

Vickers hardness was measured by using a durometer Micrometer 5103 (Buehler), loading 300 g for 10 seconds and making 30 measurements for sample.

The microstructure was studied using field emission scanning electron microscopy, FESEM (FEI: Quanta FEG 650).

The dielectric properties of the samples were studied by standard low-frequency impedance measurements (PSM1735-NumetriQ) in the 0.1Hz-1kHz frequency range.

The colour of the disks was also analysed using a spectrophotometer apparatus (Konica Minolta CM-700d model), which is based on the CIE standard light source of D65 as a light source, with a measurement area of 8 mm. The surface finish of all samples was polished down to 1µm with a sample thickness of 3 mm approximately. The final results were an average of four readings on each disk.

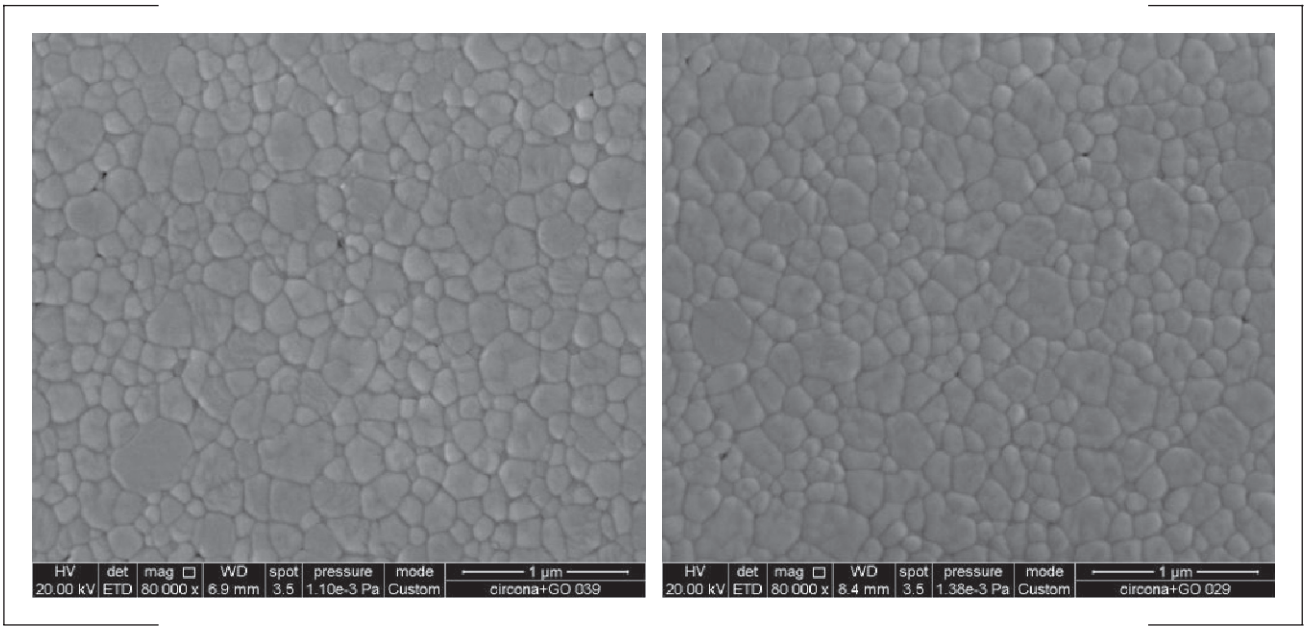
Results and Discussion

Microstructure

One of the well-known problems when reduced graphene oxide is directly used as the second phase in hydrophilic matrices, as it is the case of ceramic oxides, is the strong tendency to form aggregates due to its hydrophobic nature. As it was previously observed in the case of alumina+graphene oxide (22) in our case both components have polar surfaces favouring an electrostatic interaction between them consequently a perfect dispersions of both components (3YTZP, Graphene oxide) were reached. Additionally, these mixtures can be processed in water.

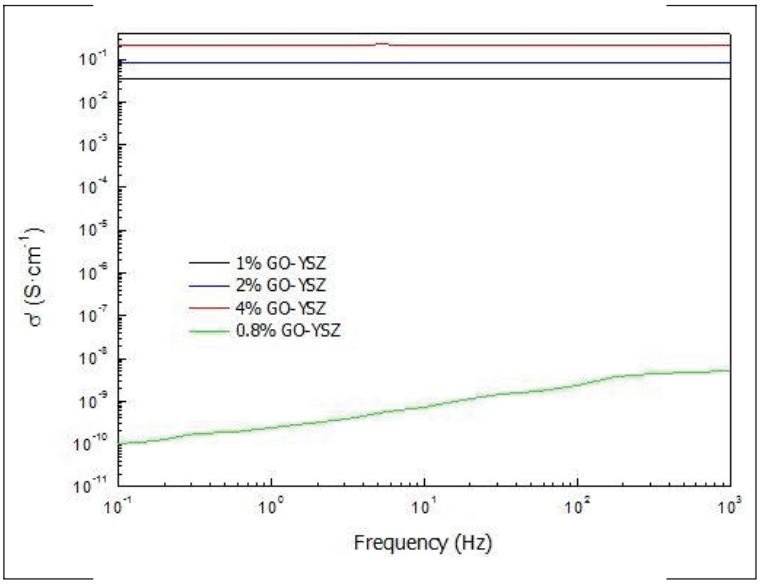
Addition of carbon second phases to ceramics have from a processing point of view several effects. Thus, during the powder packing step at the beginning of the SPS process, the graphene oxide sheets can acts as lubricant favouring the appropriate zirconia grains sliding to reach the optimum packing. Nevertheless, the incorporation of carbon second phases will difficult the composite densification. In this sense, Spark Plasma Sintering technique that applies pressure while heating is a very suitable technology for preparing this type of composites. Sintering temperature was selected by following the piston displacement during heating until the piston movement was stopped. In Figure 1 the microstructures of zirconia composites with 0, 0,29 and 0,39 wt% graphene oxide contents as examples are shown.

Figure 1 Microstructures of ZrO_2-(0,29wt%)GO (left) and ZrO_2-(0,39wt%)GO (right) composites



SPS process is carried out in reducing conditions, vacuum and graphite environment and the GO is reduced to pure graphene (22). The zirconia grain size on the microstructure of the zirconia + graphene SPS compacts is significantly affected by the presence of graphene. Graphene is not observed due to the low content added but its presence is inferred from its pinning effect on zirconia grain boundaries avoiding grain growth. Completely dense materials are obtained being the average grain size of zirconia very similar to the starting powder with biggest grains below 0,5 µm. Then, small additions of GO (<0,5 wt%) in combination with Spark Plasma Sintering allow obtaining dense materials without significant grain growth.

Figure 2 Low frequency conductivity of ZrO_2-graphene composites.



Electrical properties

In Figure 2 it is represented the electrical conductivity of ZrO2-graphene composites

It is clearly shown that the percolation threshold takes place between 0.8 and 1 wt% graphene oxide. Samples with graphene contents below 1 wt% graphene (only 0.8 wt% graphene is shown for clarity) show conductivity values close to that

of the pure YSZ whereas a gap of 8 orders of magnitude in conductivity is found on increasing the graphene content up to 1 %. The electrical behaviour of percolated samples is also different from un-percolated samples. Percolated samples show a conductivity plateau which corresponds to the dc conductivity of the percolated graphene network whereas the conductivity of the un-percolated samples increases with the frequency due to polarization between neighbouring conductive clusters. Over 1% graphene content, the conductivity of the samples gradually increases, but in much smaller gaps due to the increase of the vol. content of the conductive phase. Then, it has been determined that the minimum content for reaching the necessary low resistivity to be machined by using EDM technologies is around 1wt%. We will see now that the mechanical properties of the obtained zirconia + graphene SPS compacts with a so low content of GO addition in order to be electrical conductive are not significantly affected.

Physical and Mechanical properties

Table 1, shows the density and Vickers Hardness of ZrO2-GO composites.

Table 1. Density and hardness of ZrO2-graphene composites

	GO content (wt%)			
	0	0.3	0.4	1.0
Density (g/cm^3)	6.01	6.02	6.00	6.01
Hardness H_{v10} (GPa)	12.97	12.44	12.56	12.50

ZrO2-Graphene composites show slightly lower hardness values than monolithic zirconia. This can be attributed to the presence of a carbon phase that is a comparatively a softer material. However, the difference can be considered in the range of the error bars of the measurement.

Colour properties

Finally, blackness measurements were carried out comparing three samples; pure 3Y-TZP zirconia (“white” zirconia), commercial “black” zirconia from Tosoh and 3Y-TZP-1wt%-GO composite. In Table 2 they are shown the values obtained for L* a* b* parameters.

Table 2. Whiteness index of zirconia–GO composite in comparison with commercial white and black zirconia

	L	a	B
Commercial “White” zirconia	88,56	0,14	2,15
Commercial “Black” zirconia	44,39	0,01	-0,96
ZrO2-1wt%GO composite	36,44	0,23	0,57

The value of ΔL is increased in 18% when it is compared with the commercial black zirconia that is obtained by addition of Co_3O_4.

In summary these new family of zirconia-graphene nanocomposites are full dense materials, free of metals (Co, Fe), they reach a blackness value better than commercial black zirconia materials preserving zirconia hardness and they open the possibility to be machined by EDM thanks to their low electrical resistivity. Consequently they could be found a great number of new applications including wear resistant components as well as in the field of biomaterials were complex shaped components are required.

Conclusions

Black zirconia with blackness index higher than commercial products based on metals can be obtained by small addition of graphene. The low content in graphene allows maintaining mechanical properties of zirconia such as hardness.

Graphene-zirconia composites can be easily processed by starting form graphene oxide and performing reduction in-situ during Spark Plasma Sintering. When the graphene content is increased up to 1 wt%, electrical resistivity of composite is lower than 100 Ωcm that allows using electrodischarge machining for preparing complex shapes from these materials that are demanded for many applications fields.

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Horizons of application of nanostructured metals in medicine

ABSTRACT

Market research showed that despite the high cost of bulk nanostructured materials produced by the SPD techniques, their application in medicine is of great interest. This is due to high biomechanical properties of nanomaterials and, hence the possibility to fabricate high-strength designs with reduced weight and size parameters. The development of innovative ideas in the field of nanomaterials' application in medicine offers the challenge of performing scientific and applied work in order to develop wires, plates and other semi-products of nanostructured metals.

KEYWORDS

Nanomaterials, medical implants.

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Electrodeposited metal materials with developed surface for catalytic applications

ABSTRACT

We discuss the original methods for the creation of the metal materials with developed surface based on icosahedral small particles (ISPs). We study individual ISPs, coatings and bulk materials made of ISPs. The basic physical idea of the approach consists in the transformation of the stored in ISPs internal energy into the energy of the developed surface. Structural phase transformations and evolution of surface morphology of ISPs and materials based on them in temperature fields and aggressive environments, is discussed in details.

KEYWORDS

Developed surface, electrodeposition, metal microparticels, catalysis.

ACKNOWLEDGEMENTS

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SUMMARY

Metal materials with developed surface are widely used as catalysts, filters, sorbent materials in chemical, gas, and petrochemical technologies, water treatment and disposal, as well as in other industries. In particular, 90% of chemical goods in the World is made using catalysts, the production of which has now reached 800000 tons per year.

One of the most important characteristics of such materials is the specific surface area. It strongly influeneces the catalytic activity and sorption capacity of the material. Therefore, the development and production of metals and their oxides with a developed surface is an actual problem.

In this report, we discuss the original methods for the creation of the metal materials with developed surface based on icosahedral small particles (ISPs). We study individual ISPs, coatings and bulk materials made of ISPs [1-3]. The basic physical idea of the approach consists in the transformation of the stored in ISPs internal energy into the energy of the developed surface. Structural phase transformations and evolution of surface morphology of ISPs and materials based on them in temperature fields and aggressive environments, is discussed in details [4-6].

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Spark plasma sintering of transparent aluminum oxynitride

ABSTRACT

We studied the possibility of spark-plasma sintering aluminum oxynitride, the optimal modes and parameters of compaction. Plotted the properties of sintered samples of the temperature, pressure and dwell time. Effect of the composition on the physical and mechanical characteristics of the samples were determined. Detected factors affecting the transparency of the finished products, and the ways that allow to obtain a high light transmittance.

KEYWORDS

Aluminum oxynitride, ALON, spark -plasma sintering, transparency, structural condition, micro-hardness, mechanical properties.

SUMMARY

Development and modernization of small arms for the army makes it necessary to develop means of body armor. In particular, improved mechanical properties required of transparent armor materials used as armored glass. The most promising material for transparent ceramic armor is based on aluminum oxynitride (ALON).

Ranked among presented in the present time of ceramics, with an average density of aluminum oxynitride has a sufficiently high strength comparable to the YAG (yttrium aluminum garnet) and cubic zirconia (stabilized zirconia). And the most important characteristic for body armor - toughness - ALON surpasses all transparent materials (including quartz glass - fused quartz, spinel and leucosapphire).

Typically made from aluminum oxynitride powder mixtures of aluminum oxide and aluminum nitride. To obtain the required mechanical and physical properties of the

resulting material required density, as close as possible to the theoretical. It is also important to obtain a single-phase structure. Any inhomogeneity and second phases prevent light transmission.

To achieve the desired properties is also very important to make the preparation of raw material: powders of Al2O3 and AlN. In preparation for sintering powders may include: grinding in ball mills, and other, stirring, in a liquid dispersion and drying. Also important is the initial state and powder parameters such as particle size, purity, etc.

In this paper, attention is paid to the use of spark-plasma sintering to obtain transparent ceramics based on aluminum oxynitride, as well as the study of powder sintering cooking modes.

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The microstructure and mechanical properties promising alloys Mg-Zn-Ca system

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ABSTRACT

At present work have shown that a coarse intermetallic particles in the microstructure of magnesium alloys (Mg-Zn-Ca system) has no significant effect on fatigue crack initiation in low cycle fatigue test mode. The fatigue life of biodegradable magnesium alloys ZX50 and WZ21 after extrusion have shown comparable high-strength results in high cycle fatigue tests conducted in air atmosphere, like extruded magnesium ZK60 alloy.

KEYWORDS

Magnesium alloys; biocompatibility; mechanical properties; microstructure, corrosion fatigue.

ACKNOWLEDGEMENTS

This work was supported by the Russian Science Foundation, grant № 15-19-30025.

SUMMARY

Now there is active development of new magnesium alloys for medical purposes, around the world. Magnesium has the basic qualities necessary for biomedical applications such as biocompatibility, non-toxicity and the non-carcinogenic. An important advantage is that magnesium can fully dissolve in the body without harm. As a result, the natural corrosion of the implant in a physiological environment of the need for re-operation was not require. However, biomedical magnesium alloys, which are used as bone implants should have a sufficient level of mechanical properties, which cannot provide the pure magnesium.

Using deformation hardening methods can improve mechanical properties of magnesium alloys. Applying of severe plastic deformation (SPD) contributes high effective deformation in the workpiece and provides a mechanism of dynamic recrystallization. All this allows managing the microstructure by creating the crushed grain and the necessary distribution of secondary phases in the alloy.

Determination of fatigue properties plays an important role at the stage of detail's designing, because it affects the prediction of detail's working capacity.

The objects of study in this work are the alloys Mg-Zn-Ca system, because zinc and calcium are completely biocompatible with the human body. Furthermore, these elements in the alloy composition improve its properties. Thus, zinc is ef-

ficiently improves the mechanical properties of magnesium alloys, calcium contributes to the corrosion resistance.

All investigated alloys in this work are presented in Table 1. It should be noted that the zinc content at the level of 4-5% chosen because the higher concentration of this element in the alloy, lowers the resistance to corrosion.

At first the microstructure of the alloys with the base Mg-4Zn was investigated in the cast state. In the microstructure of these alloys in addition to the solid solution grains α-Mg, was discovered a network of intermetallic particles that are the $Ca_2Mg_6Zn_{23}$ for alloys with calcium and Mg_7Zn_3 for non-calcium alloy.

After deformation hardening of alloy microstructure U3 (Mg-4Zn) has the most homogeneous structure with an average grain size (9 ÷ 10 microns). There is no inclusion in the alloy, so it means that zinc is in a solid solution. This homogeneity of structure in comparison with the alloys U1 (0,16Ca) and U2 (0,56Ca) is reached by multiple isothermal forging after just a single pass by ECAP.

The heterogeneity of microstructure after thermomechanical processing for all other alloys observed to a greater or lesser extent. Therefore, the microstructure of alloys is bimodal, where presented both relatively small grains and large non-recrystallized grains.

Tables 1. Chemical composition and thermomechanical treatment

Alloy	Chemical composition	Thermomechanical treatment
U1	Mg-4Zn-0.16Ca	Homogenizing annealing (330°C, 10 h.) + ECAP, 1Bc, 120°, 320°C)
U2	Mg-4Zn-0.56Ca	
U3	Mg-4Zn	Homogenizing annealing (330°C, 10 h.+460°C, 7 h.) + ECAP ,1 Bc, 120°, 320°C+ MIF 2 pass 300 °C
ZX50	Mg-5Zn-0.25Ca	Homogenizing annealing (350°C, 12 h.) + extrusion (325 °C, 25:1)
WZ21	Mg-1.65Y-0.85Zn-0.25Ca	Homogenizing annealing (350°C, 12 h.) + extrusion (325 °C, 30:1)

Analysis of experiments on high-cycle fatigue results, in the air atmosphere, revealed that the extruded alloys ZX50 and WZ21 show fatigue life's properties like extruded ZK60 alloy, which is used as a reference material (table. 2). ZK60 is a bioalloy and high-strength structural magnesium alloy at the same time. It is important to note that ZX50 and WZ21 alloys after thermomechanical treatment can be attributed in the category of high-strength alloys, under fatigue characteristic

Were also performed cyclic testing of these alloys in a corrosive medical saline – 0.9 NaCl. A solution of 0.9NaCl simulates the human body solution. All samples have shown low rates of corrosion fatigue, even despite the fact that the corrosion rates of alloys samples was considerably different. Of course, the deterioration of fatigue properties was expected initially, but not to that extent.

Tables 2. Fatigue limit at cycle fatigue

Alloy	Chemical composition	Fatigue limit, MPa
U2	Mg-4Zn-0.56Ca	55
ZX50	Mg-5Zn-0.25Ca	90
WZ21	Mg-1.65Y-0.85Zn-0.25Ca	90
ZK60 [1]	extruded Mg-6Zn-0,5Zr	89,5

Fractographic research of magnesium alloys were carried out on samples after low-cycle fatigue.

By studying the fatigue failure morphology near fracture nucleus, we can conclude that the crack initiation not connected with any superficial or micro structured defect's. These intermetallic particles are present predominantly in the unstable crack growth zone and of rupture zone. So, it's do not main affect the initiation of fatigue crack.

The initiation of fatigue crack and zone of stable crack growth are only quantitative, but not a qualitative difference. The surface of fracture is formed the mechanisms of brittle fracture to form a fine structure "serrated river line", in these zones.

The unstable crack growth zone has much more developed relief, as compared with the previous stages of fracture. The presence in this zone of dimples relief, formed by the merger of micropores indicates the ductile fracture behavior of the sample in the final stages of destruction.

After high-cycle fatigue testing in 0.9% NaCl environment the fracture surface of samples heavily covered with corrosion products. In this case uniquely identify characteristic regions of fatigue fracture is not possible.

Great influence on the geometry of the sample and the fracture has a load at which the test takes place. Thus, the section geometry of alloy samples tested under high loads (50 MPa), varies significantly under the influence of a corrosive medium. The cross section of samples is rounded only slightly (Fig. 1a), but he is still rectangular. Whereas a samples tested at low loads (25 MPa) in a corrosive environment is acquire virtually circular cross section (Fig. 1b).

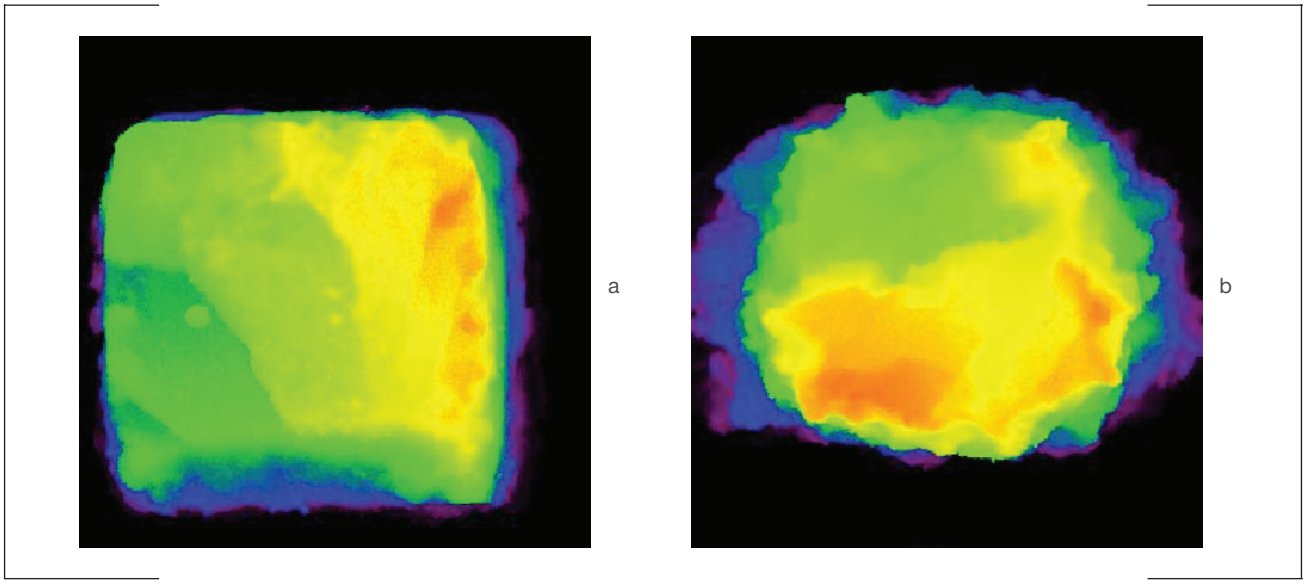

Figure 1 - A typical view of the fracture surface of the samples after fatigue testing in corrosive environment 0.9NaCl by the example alloy ZX50, tests under load:
a - 50 MPa, b - 25 MPa

Most probably, this is due to with the fact that the sample is longer in corrosion environment at low loads. Thus, the role of corrosion in cyclic tests is reduce the cross section of the sample during the experiment, which leads to a working stress increase. The high corrosion rate is a decisive factor in the degradation of mechanical properties during cyclic tests.

Conclusions

1. Microstructure is heterogeneity after thermomechanical processing observed to a greater or lesser extent. The most homogeneous microstructure achieved after multiple isothermal forging (alloy U3).
2. The best characteristics of fatigue in the air have extruded alloys ZX50 and WZ21.
3. The particles of secondary phases in the alloys U1 and U2 do not substantially affect the mechanical properties, including fatigue failure.

Special thanks go to M. Linderov for his careful LCF and HCF experiments.

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Femtosecond laser modification of silver doped zinc-phosphate glass

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ABSTRACT

A high silver-content zinc-phosphate optically transparent glass was modified by femtosecond laser. Micron-sized donut-like structures were formed in the volume of glass. Silver nanoparticles showing surface plasmon resonance effect and intense luminescence were formed on the edges of the structures while birefringent regions were formed in its center. Independent control of luminescence and birefringent in such structures could pave the way for the 6D optical data storage in glass.

KEYWORDS

Zinc-phosphate glass, femtosecond laser modification, silver nanoparticles, birefringent nanogratings.

ACKNOWLEDGEMENTS

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SUMMARY

Using of ultrafast and highly intense laser sources open routes for precise space-selective tuning of properties of the solid matter that can be used for design of nanocomposite and nanostructured materials. Among other techniques, femtosecond laser modification (FLM) represents a maskless patterning process that provides rapid patterning at sub-micrometer resolutions with flexibility, ease of use, and cost effectiveness [1].

FLM process is most widely used for patterning of optical materials (crystals, polymers and glasses) due to non-linear character of light-matter interactions providing high space selectivity. Significant results in channel waveguides formation and bulk precipitation of metal nanoparticles and nonlinear crystals were achieved during past decades [1]. One of the especially important applications of FLM process is the realization of approach for the 3D optical data storage in glass. This approach potentially enables dramatical increase of data storage density and lifetime. Different parameters of laser modified areas of glass can be used for data encoding (refraction index change, retardance and slow axis of birefringent nanogratings, luminescence of metal nanoclusters etc.) [2, 3]. Formation of birefringent nanogratings was widely demonstrated in fused silica glass and couple of silicate glasses [2]. At the moment, one of the most attractive materials for initiation of light emitting centers in the bulk of glasses is phosphate glass containing photosensitive agents such as noble metals (Ag, Au) [3]. Glass interactions with highly intense laser pulse leads to spatially selected precipitation of metal nanoclusters or nanoparticles which can exhibit luminescence in the visible region. Despite of existence of studies of these parameters alone it is a lack of studies for simultaneous formation in glass both birefringent nanogratings and luminescent emitters that could potentially lead to increase of recording density. The present study reports the possibility of simultaneous formation of silver nanoparticles and birefringent regions in the volume of phosphate glass by means of femtosecond laser modification.

Silver-doped glass preparation was achieved by the melt-quenching technique for a zinc-phosphate glass matrix of 40P2O5-55ZnO-4Ag2O-1Ga2O3 composition (mol.%). The obtained glass was transparent and optically homogeneous. A setup equipped with NIR femtosecond laser (Nd:YAG, 6W, 100 kHz, 600 fs at 1030 nm, Pharos SP by Light Conversion Ltd.; Olympus objective LCPLNIR 50X NA 0.65) and a high-precision 3D translation stage (Aerotech ABL1000) was used for FLM. Micron sized dots with 10 μm spacing were written by the laser beam about 45 μm below the glass surface. FLM was performed for different laser pulse energies from 38 to 73 nJ and different number of pulses from 1,3 to 10,4 x10^5. For each

energy and number of pulses a laser beam polarization angle was varied for 0, 36, 62, 98, 144 degrees relative to the starting position by means of a half-wave plate. Quantitative analysis of birefringence was performed by CRi Abrio system installed in the optical microscope Olympus BX61. Luminescence analysis was carried out using Nikon Eclipse Ni-E epifluorescence microscope.

As a result, a set of donut-like dots from 3 to 5 μm in diameter increasing with the energy and number of applied laser pulses was formed. The dots had yellowish colour at the edges and were colorless and transparent in the center. The fluorescence microscopy with excitation at 380 nm revealed the noticeable luminescence appearing on the edges of modified regions. Yellow coloration of the edges is the indirect evidence of silver nanoparticle formation due to FLM of glass. Thus, to confirm that fact, a set of 100 μm long lines with the width of 5 μm immediately adjacent to each other was written resulting in yellow coloured rectangular area inside the glass. Absorption microscpectroscopy was performed both in laser modified area of the glass and outside this area revealing the absorption band with a maximum at 445 nm associated with surface plasmon resonance of silver nanoparticles. This clearly confirms the formation of silver nanoparticles in the bulk of the phosphate glass due to FLM. A mean size of nanoparticles calculated in terms of Mie theory was about 3-4 nm. On the other hand, clear observed luminescence from the edges of donut-like dots indicates the presence of silver nanoclusters. Thereby it can be assumed that silver aggregates with a wide size distribution including both plasmonic silver nanoparticles and luminescent silver nanoclusters formed during the FLM of zinc-phosphate glass.

At the same time, birefringence was clearly observed in the central regions of donut-like dots along with nanoparticles and nanoclusters formation in the edges of dots. The retardance measured after glass irradiation by 2,6x10^5 laser pulses was about 10 nm. Increasing the number of pulses up to 10^6 resulted in the increase of retardance up to 30 nm in the center of dot. It should be noted that the slow axis orientation in the birefringent areas correlated to the linear polatization of the applied femtosecond laser beam being always perpendicular to its polarization plane. This case is typical for birefringent nanogratings in glass and gives and indirectly indicates of appearance of nanogratings which were not reported in phosphate glasses earlier.

In conclusion, possibility of simultaneous formation of both luminescent silver nanoparticles and nanoclusters and birefringence nanogratings in the bulk of silver doped zinc-phosphate glass by femtosecond laser modification has been demonstrated. Further study is going on to show the possibility of independent control of birefringence and luminescence by means of varying the irradiation conditions. This may open the way for the multilevel encoding for data recording in silver doped zinc-phosphate glass.

This work was financially supported by the Ministry of Education and Science of the Russian Federation (grant 14.Z50.31.0009), the Grants Council of the President of Russian Federation (grant MK-9290.2016.3) and the Russian Foundation of Basic Research (grant 16-03-00541).

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Self-propagating high-temperature synthesis of Ni2AlTi

SCIENTIFIC ORGANIZATION

National University of Science and Technology MISiS

ABSTRACT

We have investigated obtaining of the Ni2AlTi compound using SHS, which is a cheap and environmentally friendly method of this material producing; obtained Ni2AlTi compound. In the present study parameters for obtaining of single-phase samples were established for using of self-propagating high-temperature synthesis in argon atmosphere, where initiation of self-propagating reaction was provided by tungsten wire. The parameters of obtaining more than 90% dense samples using spark plasma sintering and hot pressing were investigated also.

KEYWORDS

Self-propagating high-temperature sythesis, combustion synthesis, NiAl-based alloys, spark plasma sintering, hot pressing.

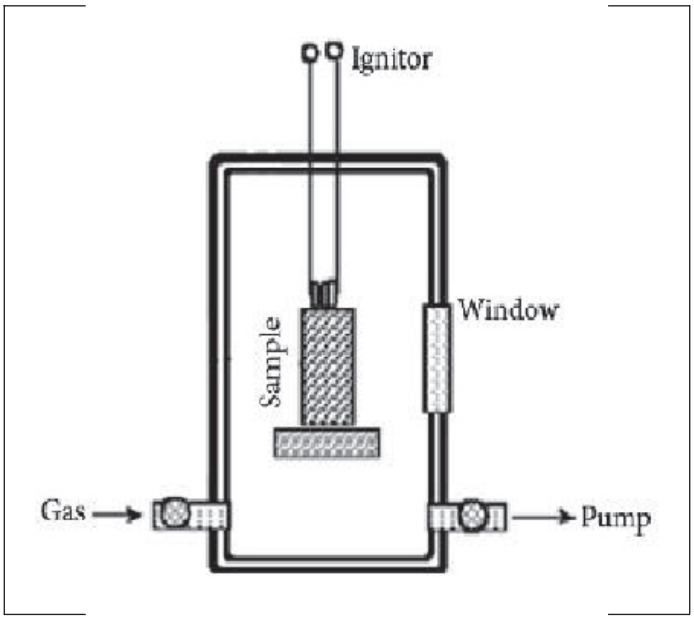


Figure 1. Schematic of SHS reactor

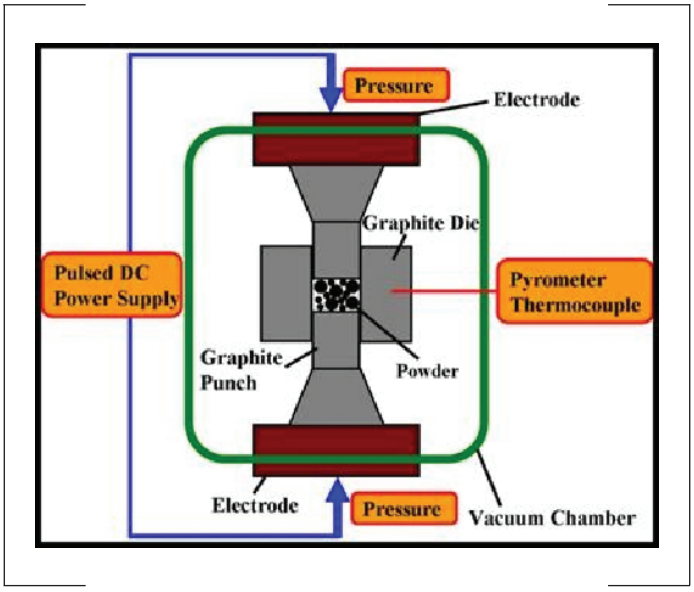


Figure 2. Schematic of spark plasma sintering system

ACKNOWLEDGEMENTS

I am very grateful to prof. A.S. Rogachev, prof. A.S. Mukasyan, prof. I.A. Abrikosov and Ph.D. D.O. Moskovskikh for their support in carrying out of this work.

SUMMARY

Self-propagating high-temperature synthesis (SHS) is a method for producing inorganic compounds by exothermic reactions, usually involving salts or pure metals. A variant of this method is known as solid state reactions. Since the process occurs at high temperatures, the method is ideally suited for the production of refractory materials with unusual properties, for example: powders, metallic alloys, or ceramics with high purity, corrosion–resistance at high–temperature or super-hardnessity. Self-propagating high-temperature synthesis (SHS), also known as combustion synthesis (CS), is an energy saving technology to fabricate NiAl-based alloys [1].

The intermetallic nickel aluminide compounds have several exciting features, including low-density, high melting point, excellent corrosion and oxidation resistances, high strength at increased temperature and relatively low cost [2]. For these reasons, these intermetallics are good candidate for diversity of application as elements for airframe and turbines [3]. It was also known that these compounds possess low ductility and tendency for brittle fracture, especially in polycrystalline form, which limited their applications [4]. The alloying, which involves different dopants, such as B, C, Ti, Zr, Nb and Ta, has been used to overcome the problem [5].

In this work were used several methods of SHS:

- direct SHS in argon atmosphere, where initiation of self-propagating reaction was provided by tungsten wire (Fig 1);
- direct SHS of mechanical activated powder mixture;
- spark plasma sintering of mechanical activated powder mixture (Fig 2);
- hot pressing of synthesized material.

The following powders were used to synthesized materials: aluminum (ASD-1); nickel (PNE-1); titanium (PTS-1). The powders were thoroughly mixed to prepare heterogeneous mixtures, which correspond to required composition (see Table 1).

Table 1. Compositions of used powder mixtures

Compound	Metal	Amount of metal, wt.%
Ni2AlTi	Ni	61,1
	Al	24,9
	Ti	14,0

Prepared mixtures were pressed in the uniaxial press dye to form a cylindrical samples (d=15mm; height = 5 mm) to the density 3,4 g/cm^3. Fabrication of the intermetallics was performed by using self-propagating high-temperature synthesis method. The basic idea is that the reaction between Al and Ni is extremely exothermic with adiabatic combustion temperature ~1911 K [6]. It means that if one locally (~1 mm^3) preheat the mixture to some temperature reaction initiates and propagates in the self-sustained manner along the bulk of the sample, forming desired intermetallic phase. In our case, the samples were inserted into the stainless steel reactor, which was first pumped down to vacuum ~ 10^{-3} Pa and then filled with argon gas to the pressure of ~ 0.5 MPa. The local preheating of the sample was accomplished with the electrically heated tungsten wire.

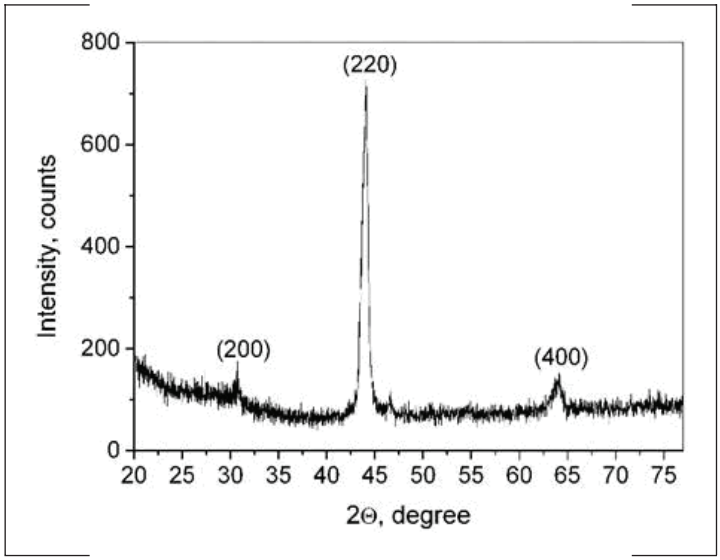


Figure 3. Diffraction pattern of synthesized sample

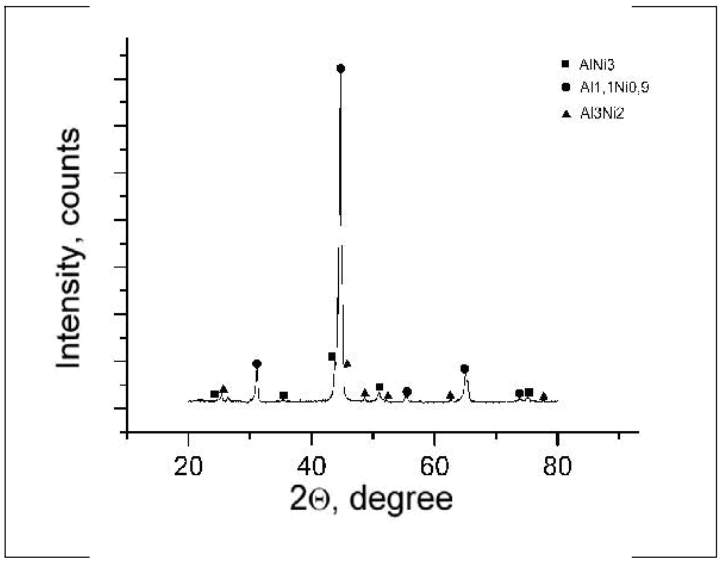
In presented work for mechanical activation was used high-energy ball mill «Activator 2S» («Activator», Novosibirsk). For sintering was used spark plasma sintering system «LABOX Model-650».

Also phase composition of prepared samples were studied by x-ray diffraction analysis (DRON-3).

The diffraction pattern of samples obtained by SHS represented on figure 3. It is obvious that able to obtain single-phase samples by the method. However, the samples had a very low density (~35-50%). In order to avoid this, we used the methods following below.

The next step of researching synthesis of Ni2AlTi was SHS of pretreated by mechanical activation powder mixture. For this operation we have used high-energy planetary ball milling (694 rpm, 2 minutes). Mechanical activation provides a denser samples by the increase contact area between the particles and reduce the distance between the particles of the reaction mixture. The obtained samples had a higher density of around 70% with single-phase composition, such as non-activated samples.

Figure 4. Diffraction pattern of sample obtained by spark plasma sintering



However, this density is not sufficient for the material application. Cylindrical samples (15x6 mm) obtained by the spark plasma sintering of pretreated with mechanical activation reaction mixture. Diffraction pattern of this samples is presented on figure 4. The sintering temperature was 800oC, the dwell time - 10 min, pressure - 40 MPa.

The temperature was then increased and the other parameters remained unchanged. At a temperature of 900oC was able to get single-phase samples (density ~ 90%).Supposedly it is caused by the alpha - beta phase transition in titanium that provides extra warmth over the entire volume of the sample and creates favorable conditions for the synthesis process.

The powder mixture directly synthesized by SHS was used for the densest samples sintering by hot pressing. These samples have a relative density of ~ 93-95 %. Sintering parameters are presented in Table 2.

Table 2. Hot pressing parametrs

Temperature, °C	1200
Pressure, MPa	40
Dwell time, min	10
Heating rate, °C/min	100

This confirms the fact that this method allows to obtain a consolidated material suitable for further use.

Conclusions:

- We have investigated obtaining of the Ni_2AlTi compound using SHS, which is a cheap and environmentally friendly method of this material producing;
- obtained Ni_2AlTi compound;
- parameters for obtaining of single-phase samples were established for using of self-propagating high-temperature synthesis in argon atmosphere, where initiation of self-propagating reaction was provided by tungsten wire;
- the parameters of obtaining more than 90% relatively dense samples using spark plasma sintering and hot pressing were investigated also.

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SCIENTIFIC ORGANIZATION

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Characterization of Picoscale 3D Local Atomic Structure of Nanomaterials by High Energy Resolution Synchrotron Based XANES Spectroscopy

ABSTRACT

Novel in-situ technique for picoscale characterization - extracting of 3D local atomic structure parameters on the basis of advanced quantitative analysis of X-ray absorption near edge structure (XANES) and high energy resolution XANES - has been developed. The possibility to extract information on bond angles and bond-lengths (with accuracy up to 1 pm) is demonstrated.

KEYWORDS

Nanocience, novel materials, nanodiagnostics, synchrotron radiation.

ACKNOWLEDGEMENTS

The research is supported by the Mega-grant (Agreement 14.Y26.31.0001) of the Russian Federation Government to support scientific research under the supervision of leading scientist and by Southern Federal University of Russia.

SUMMARY

The study of nanoscale atomic structure of matter is important both from fundamental point of view for the understanding the nature of physical and chemical properties of the materials and for applied research as a basis for the synthesis of novel nanomaterials with necessary properties, for example, advanced nanocatalysts based on metal clusters functionalized MOF and zeolite class family materials. To gain deep insight into the nature of the relation “structure-function” one has to use both computer nanodesign and advanced experimental methods for nanodiagnostics. The status of modern theoretical analysis of the experimental x-ray absorption spectra to extract structural parameters is presented.

Novel *in-situ* technique for picoscale characterization - extracting of 3D local atomic structure parameters on the basis of advanced quantitative analysis of X-ray absorption near edge structure (XANES) and high energy resolution XANES - has been developed. The possibility to extract information on bond angles and bond-lengths (with accuracy up to 1 pm) is demonstrated.

In the framework of these approaches the results of recent studies of local atomic structure for several types of advanced nanomaterials are reported. The nowadays progress in the development of the synchrotron radiation facilities for time dependent measurements opened the possibilities for the study the atomic and electronic structure dynamics as well. The specific feature of the method is that it makes it possible not only determine with high precision the interatomic distances between the atoms in nanostructured materials without long range order, but also to estimate the angle distribution of atoms (chemical bond angles) and do all this for the processes lasting less than a nanosecond.

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Phosphate glasses activated with Yb3+ ions

SCIENTIFIC ORGANIZATION

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ABSTRACT

Stimulated emission cross-section of Yb3+ for phosphate glasses containing Al, Ba, K, B, Si oxides and different additives of Yb2O3 melted from reagent grade starting materials with dry oxygen bubbling, has been examined. The effect of the drying time on the content of OH- ion impurity was estimated and the optimal drying time was determined. Concentration quenching of luminescence is established to absent for Yb3+ concentration up to 8·1020 ions/cm3.

KEYWORDS

Phosphate glass, rare-earth ions, NIR luminescence.

ACKNOWLEDGEMENTS

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SUMMARY

The advantages of Yb-activated laser materials have been recognized for generation of ultra-short pulses and high peak powers [1]. In comparison to neodymium phosphate laser glasses, the use of Yb as activator has some advantages: a simple electronic structure of Yb ions avoids concentration quenching of luminescence and excited-state absorption. The relatively long fluorescence lifetime and the broad absorption and emission bands allows to consider Yb-doped glasses as attractive material for generation of ultra short pulses and high-power pulse am-

plification. Phosphate glasses exhibit a wide transmission range, high solubility for rare earth ions, long fluorescence lifetime and tailorable properties by changes of the glass composition [2,3]. The aim of this paper is to clarify the conditions of preparation of Yb-containing phosphate glass samples with high optical quality and low concentration OH- ions and to study their optical and luminescent properties depending on both Yb2O3 content in the range of 1 - 5 mol.% and time of dry oxygen bubbling.

Phosphate glasses with nominal compositions (100 – X) (52,2 P2O5, 8,4 BaO, 17,0 K2O, 5,35 SiO2, 9,6 Al2O3, 7,4 B2O3) + XYb2O3(X= 1÷ 5) were prepared using phosphoric acid, boric acid, aluminum hydroxide, carbonates of barium and potassium, silicon and ytterbium oxides as raw materials. All chemicals used in the synthesis were of “high pure” and “chemically pure” grade. Batches were calculated to yield 200 g of glass and were mixed homogeneously in silica glass crucible and subsequently melted in a platinum crucible at 1400 °C for about 1 h in air and up 1 to 6 hours with dry oxygen bobbling with pouring out of melt in a steel mold and finally annealing at 450÷ 550°C for 4 h. Absorption spectra, excitation and emission spectra and luminescence decay curves were recorded with the use of conventional techniques. All measurements were carried out at room temperature.

Luminescence quenching is established to absent for Yb3+ content up to $8 \cdot 10^{20}$ ions/cm3 (i.e. ~3,5 mol.% Yb2O3) that may be connected with relatively small efficiency of donor-donor energy migration in these glasses. As a result the Yb3+-activated glasses show luminescence quantum yield 93% for glasses with 1 mol% Yb2O3 and even for heavily activated glasses with 5 mol.% Yb2O3 luminescence quantum yield is higher 45%. The influence of pumping wavelengths on the lifetime of Yb3+ was also investigated and the optimal excitation wavelength for studying the kinetics of luminescence quenching was determined. The luminescence efficiency of glasses was found to be the function of not only Yb2O3 content but also glass drying time. It was shown that the glass dehumidification procedure should be continued at least 3 hours. The optimal duration of glass melt drying was determined taking into account both the absorption coefficient value at 3100 nm (absorption band of OH ions) and a change in the luminescence decay time for each Yb3+ concentration.

Achieved properties of synthesized phosphate glasses in combination with their manufacturability refer them to promising heavily doped laser materials.

This work is financially supported by the Ministry of Education and Science of the Russian Federation (grant 14.Z50.31.0009).

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Fabrication and plasma treatment of different materials for biomedical applications

SCIENTIFIC ORGANIZATION

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ABSTRACT

The prospectives of rapid printing technologies and implant surface modification strategies to prepare 2D thin films and 3D scaffolds are discussed. Low-temperature plasma processing has been shown as a very prospective way to tailor both physico-chemical and mechanical properties of metals and polymers for regenerative medicine.

KEYWORDS

3D printing, polymer and metallic scaffolds, plasma treatment, surface wettability and energy.

ACKNOWLEDGEMENTS

Federal Target Program #14.587.21.0013 (a unique application number 2015-14-588-0002-5599, project in the frames of ERA.NET RUS Plus – S&T Call, #58 INTEL-BIOCOMP), Russian President grant for young scientists Candidate of sciences #MK-6459.2016.8.

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Coherent propagating spin waves excited in nano-structures by pure spin currents

SCIENTIFIC ORGANIZATION

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ABSTRACT

Utilization of pure spin currents not accompanied by the flow of electrical charge creates novel opportunities for emerging technologies based on the use of the spin degree of freedom - spintronics and magnonics. Smaller power dissipation and utilizing insulating magnetic materials makes nano-devices based on spin current unique functional. We demonstrate a nano-system, where pure spin currents generated by the nonlocal spin injection mechanism efficiently excite spin waves in a magnonic waveguide. The construction can be used for complex magnonic integrated circuits.

KEYWORDS

Spin current, spin waves, spin-current injection, micro-Brillouin light scattering, hybrid nanostructures, magnon nano-optics, integrated magnonic devices.

ACKNOWLEDGEMENTS

The results were obtained within the grant of the Russian Ministry of Education and Science № 14.Z50.31.0025 and the state assignment of FASO of Russia (theme “Spin” No. 01201463330).

SUMMARY

Recent intense research on the interactions of pure spin current with magnetization resulted in the demonstration of novel nano-devices, where the coherent magnetization oscillations are driven by spin currents created either due to the spin-Hall effect in materials with strong spin-orbit interaction or due to the nonlocal spin injection. Utilization of pure spin currents not accompanied by the flow of electrical charge creates essentially novel opportunities for emerging technologies based on the use of the spin degree of freedom for nanoscale data storage, transmission, and procemssing, such as spintronics and magnonics. In addition to the evident

advantages of smaller power dissipation and the possibility to utilize insulating magnetic materials the absence of the requirement of electrical current flow in active magnetic layers makes nano-devices based on pure spin current uniquely flexible resulting in novel device geometries and functionalities. Recently it was shown that pure spin currents can be used to excite coherent magnetization dynamics in magnetic nano-structures. However, in all the demonstrated devices the magnetic auto-oscillations are spatially confined and do not emit propagating spin waves in the outside world, which does not allow the use of these devices as sources of traveling waves for nano-scale magnonic circuits, where spin waves play the role of the signal carrier.

We demonstrate experimentally with applying a micro-focus Brillouin light scattering spectroscopy a magnonic system driven by pure spin currents, where the above conflicting requirements are simultaneously satisfied. This is achieved by utilizing a combination of two dynamically coupled subsystems possessing different characteristics: the active subsystem where the interaction of the pure spin current with the magnetization takes place resulting in the excitation of spatially confined dynamical mode, and the spin-wave guiding subsystem, where the efficient propagation of spin waves is possible. We show that such heterogeneous systems can be implemented by using the nonlocal spin-injection spin-current generation mechanism, which allows one easily to tailor the topography of the active magnetic layer. The demonstrated system shows efficient and controllable excitation of coherent propagating spin waves with large propagation lengths and their directional transmission.

The proposed construction is amendable to modifications and can be used as a building block for complex magnonic integrated circuits.

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Nanocomposites for top-end Functional Applications: the CINN-LECAST experience

SCIENTIFIC ORGANIZATION

Stankin Moscow State Technological University

ABSTRACT

Nanocomposites entirely made of ceramic and metallic nanoscale particles, is a term that denotes a broad, new class of engineered materials where unique and otherwise unattainable properties can be revealed. The industrial applications of nanocomposites rely on the successful consolidation of these materials preserving their nanostructures. This lecture presents the accumulated experience in this field during the last 10 years at both CINN and LECAST, with special emphasis on “what we don’t know” and “questions to which we still seek answers”.

KEYWORDS

Hybrid Spark Plasma Sintering, ceramic composite materials, nanomaterialsm powder materials.

ACKNOWLEDGEMENTS

Authors would like to thank The Ministry of the Russian Federation supported this work in the frame of Governmental Regulation of the Russian Federation No. 220, 9 April 2010 by contract 14.B25.31.0012, 26 June 2013.

SUMMARY

Currently ceramics and composites are not suitable for the industrial development of many technological innovations due to the impossibility of combining in the same material high mechanical performance with critical functional material properties. Nanocomposites entirely made of ceramic and metallic nanoscale particles or nanoscale phases, is a term that denotes a broad, new class of engineered materials where unique and otherwise unattainable properties can be revealed. The industrial applications of nanocomposites rely on the successful consolidation of these materials preserving their nanostructures. Traditional processing techniques

have strong limitations of not being able to retain the nanoscale grain size if conventional nanoparticles are used as starting raw materials.

Scientific approaches to design and develop new advanced multifunctional materials in CINN and LECAST (STANKIN)

Bulk Superhard Nanocomposites

Previous experimental results of hardness of single phase nanostructured metals or metallic superlattices clearly indicate that hardness increases with decreasing grain size (below 100 nm) up to 5-7 times following a $d^{-1/2}$ dependence known as Hall-Petch effect. The origin of superhardness in these composites is attributed to the following factors: i) the suppression of dislocations due to the small crystal size of nanoparticles; ii) the supermodulus effect in the nanocrystal core due to the compressive stress of the non-crystalline shell; iii) a strong interaction in the interface between different components. In this sense, the optimization of microstructural parameters of nanocomposites is a crucial subject, which has been treated in many studies.

In order to optimize the hardness of ceramic/metal nanocomposites, it would be necessary to increase the fraction of the hard phase through increasing the ratio r^0/R (being R the radius of the matrix grain). It can be done by using ceramic matrices with very small grains. However, the sintering of such composites is not easy, considering that the growth rate of ceramic nanoparticles is very high, inducing exaggerated grain growth.

In order to overcome this roadblock, in STANKIN Megagrant project we use the singular properties of nanocrystalline metals embedded in dense rigid matrices opening a new avenue to prepare superhard materials suitable to be used for metallurgical applications where diamond-based materials do not work. The enhancement of the fraction of monodisperse nanoparticles in harder matrices can produce new superhard cermets (H>40 GPa) at reasonably low cost.

High Creep Resistant Nanocomposites

The cohesive strength and diffusion at interfaces often control engineering properties of structural materials such as hardness, yield strength, fracture toughness, creep and creep fracture, and fatigue behaviours both at low and elevated temperatures. The interface and grain boundary effects begin to dominate properties as the microstructure is reduced to the nanoscale. Therefore, the basic premise is that novel functionalities for mechanical engineering applications (hardness/strength/ductility/creep) designed into advanced nano and innovative composites by employing a suitable nanoscale or other fine scale architecture to control the properties. In this part of STANKIN Megagrant project, we seek to address the design of nanostructured and innovative nanocomposites not by just refining the polycrystalline microstructural scale, but rather by exploring how the **electrical current assisted sintering** allow as controlling the structure of grain boundaries of developed nanoceramics and ceramic-metal nanocomposite materials to achieve unusual mechanical and possibly other properties. By this way we try to fulfil the requirements of advance materials working in extreme conditions. In the case of nanoceramics, poor toughness results from the lack of dislocations and their mobility. To alleviate some of these problems, it was proposed up to now to reduce grain size. But the problem arises when these developed materials have to work at high temperatures under extreme conditions. Grain size reduction enhances grain-boundary sliding and grain-boundary diffusion related creep phenomena thereby inducing ductility at low temperatures. In the nanoscale regime, we envisage that grain-boundary sliding and creep phenomena dominate and control their mechanical properties. In our project we try to resolve this important issue by developing nanostructured nanoceramics with a bimodal grain structure in order to take profit of the nanostructure of some phases both as functional nanoparticles and as grain boundary modificators, by introducing residual stresses and by changing the nanochemistry of grain boundaries and as a consequence grain boundary diffusion rate at high temperatures.

Optical Windows

Taking into account the nature of the pore and grain scattering, the conditions to prepare transparent ceramics resumed: i) we have to use nanometer sized powders; ii) the quality of the green body must be excellent free of defects, bubbles or impurities; iii) sintering by **electrical current assisted sintering** should eliminate porosity (<0.1%) with a pore size smaller than 10 nm; iv) the resulting grain size

should be smaller than 1 micron and/or some texture with the c-axis perpendicular to the surface of the sample should be induced.

In order to attain the requisites, a series of specific steps carried out. First of all, high purity nanometer sized powders are required and have to be conditioned. They must be homogenised and subjected carefully to a forming process before sintering to avoid ambient contamination and processing defects, such as bubbles or large packing defects. The obtained green body must be thoughtfully calcined inside the mould to remove any organic residual. The subsequent sintering process by **electrical current assisted sintering** should densify the material to theoretical density, but keeping the grain size small. This later process was done by doping the starting powders with some other oxide like CeO2, that help to increase the green density and hinder the grain growth and/or change the mass transfer mechanism depending on the atmosphere (changing from Ce4+ to Ce4+).

Low thermal expansion nanocomposites

In our LECAST STANKIN laboratory we studied the phase equilibrium diagram L-A-S containing the compositions with negative CTE revealing the most desirably phases for the fabrication of the composite according to the chemical compatibility. This diagram reveal the temperature range in order to obtain dense bodies after sintering of the designed composites. And this is a key issue in this project as LAS phases with negative thermal expansion coefficient have relatively low melting points compared with silicon carbides and nitrides. Furthermore, the invariant points in the LAS system are relatively close to the pure LAS phase compositions. The temperatures of these points are with around 1000 ºC quite low. This is why the electrical current assisted sintering can be the only way to obtain dense LAS/SiC(for example) composites with tailored thermal expansion coefficient as this method can lower the sintering temperature which is a very convenient point in these systems avoiding the formation of a melted phase (glasses).

Once the most suitable compositions be chosen and the nanocomposite was be designed, it necessary to synthesize the NTE materials (LAS or cordierite). The nanocomposites was made from mixtures of these materials with second phases of nanometric size (nSiC, nSi4N3, CNF…). Especially the addition of CNF would help to improve the requirements of electrical conductivity. CNF also help to get better thermal diffusivity if the amount and dispersion of this component in the matrix of the nanocomposite is under control.

Once dense nanocomposites are obtained, they was be characterized from the physicochemical and structural point of view. It is mandatory to get to a final compromise between the CTE values of the composites and their mechanical properties in order to obtain a suitable material for the functional final application.

ADDITIONAL INFORMATION

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Bulk Nanostructured Materials with Superior Properties for Innovation Applications

SCIENTIFIC ORGANIZATION

Ufa State Aviation Technical University

SUMMARY

In recent years the development of bulk nanostructured metallic materials has become one of the most topical directions in modern materials science. Nanostructuring of metals and alloys paves the way to obtaining unusual properties that are very attractive for innovative applications [1, 2]. In this research topic, the use of severe plastic deformation (SPD) techniques attracts special attention since it offers new opportunities for developing new technologies of fabrication of various large semi-products from nanostructured materials in the form of sheets, rods, thin foils, wire, for various specific applications [2, 3]. Recent years also witness the transition of SPD methods such as high pressure torsion (HPT), equal channel angular pressing (ECAP) and others from laboratory scale to commercial techniques

based on continuous processes, for example ECAP-Conform. These new trends are considered with details in the present lecture.

Especially significant progress has been made recently in the development of physical principles of enhancement of nanomaterials properties. It is well-known that nanostructured metals and alloys very often demonstrate high strength at the expense of ductility and may even be brittle, which hinders their wide application as structural materials.

We demonstrate in this talk that application of grain boundary (GB) engineering principles, i.e. generation of mostly high-angle grain boundaries with nonequilibrium, strain-distorted structure [4] or formation of GB segregations and precipitations makes it possible to achieve unique combination of multifunctional properties in nanomaterials [5, 6]. As a result we can produce the materials with high fatigue strength, endurance, increased fracture toughness. The examples of successful realization of these principles applied to enhance the properties in a number of commercial alloys based on Al, Ti and steels are given in the report. Also first pilot articles for innovative applications in medicine and engineering as well as ways of their commercialization are considered and discussed.

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Vikharev Anatoly
Doctor of Science
Head of Department

Semiconductor CVD diamond for electronic devices

SCIENTIFIC ORGANIZATION

Institute of Applied Physics RAS

ABSTRACT

A.L. Vikharev and J.E. Butler Institute of Applied Physics, Russian Academy of Sciences, Nizhny Novgorod, Russia.

KEYWORDS

CVD diamond, boron doped diamond, delta doping, diamond electronics.

SUMMARY

One of the strategies for enabling active electronic devices based on diamond is ‘delta doping’ with an electronically active impurity dopant (donor or acceptor). This strategy is proposed as a mechanism to overcome the high thermal activation energy of the known electronically active dopants, boron (0.32 to 0.37 eV) and phosphorous (05 to 0.6 eV) to create electronically mobile carriers (holes in the valance band or electrons in the conduction band) without sacrificing the mobility penalty resulting from heavily doped material. This concept of delta doping of dia-

mond with boron was investigated in Diamond electronic laboratory organized for carrying out of grant “Semiconductor CVD diamond for high-power and high-frequency electronic devices” in Institute of Applied Physics of the Russian Academy of Sciences and in collaboration with St. Petersburg Electrotechnical University (LETI). Initial Hall effect measurements of the carrier concentrations and mobility of the holes indicates successful ‘delta doping’. We have designed and constructed a unique microwave plasma driven chemical vapor deposition reactor built solely for the purpose of delta doping. Key features of this reactor are an ultra-rapid reactant gas switching system, high velocity laminar flow, independent control of substrate temperature. Also, extreme care is taken to substrate preparation, quality and roughness. We report here our strategy to achieve successful delta doping of diamond with boron and initial electrical characterization of our delta layers with results better than that achieved by previous researchers. Also designs of some electronic devices based on this material are discussed.

Voronin Denis
Dr.
Senior researcher

In vitro and in vivo visualization and trapping of fluorescent magnetic microcapsules in a blood stream

SCIENTIFIC ORGANIZATION

Saratov state university

ABSTRACT

We report on in vitro and in vivo trapping of fluorescent magnetic microcapsules in a whole blood stream. First, we optimized the capsules composition to detect florescence in a blood. Afterwards, we designed an experimental setup that allowed real-time observation of the capsules in a blood stream. The next step was in vitro trapping of the capsules in a glass vessel. Finally, we trapped the capsules in vivo in a rat mesentery blood vessel by magnetic field applied downstream from the injection place. This approach may be promising for targeted delivery systems for cancer therapy.

KEYWORDS

Drug delivery, polyelectroly microcapsules, non-uniform magnetic filed, in vivo manipulation.

ACKNOWLEDGEMENTS

The study was supported by the Government of Russian Federation (grant № 14.Z50.31.0004 to support scientific research projects implemented under the supervision of leading scientists at Russian institutions and Russian institutions of higher education).

SUMMARY

At last few decades polyelectrolyte microcapsules were shown as promising candidates for targeted delivery and remote controlled release of encapsulated drugs. The main benefits of polyelectrolyte microcapsules comparing to other delivery systems are high loading capacity and adjustability of physical and chemical properties. Typical capsules size is in a micrometer range that allows an effective loading of various compounds in capsules cavity. Capsules are prepared by stepwise deposition of charged species so that different polymers and inorganic nanoparticles can be used as building blocks bringing the functional properties and responsibility to external stimuli. However, to put into practice the capsules as a targeted delivery system one should realize their behavior in a body and have the ability to localize the capsules in the desired area. A number of publications shows that incorporation of magnetic nanoparticles into capsules shell makes them sensitive to external magnetic field. From this point, the non-uniform magnetic field seems to be perspective for accumulation of magnetic microcapsules, for instance, injected in a blood vessel feeding a tumor. Thus, it is essential to design the capsules so as to distinguish them from the whole blood environment as well as to be able to trap them via gradient of magnetic field.

In this work we would like to report about our results on in vitro and in vivo trapping of fluorescent magnetic microcapsules in a whole blood stream. The first part of this work was devoted to optimization of capsules composition in order to detect florescence in a blood. Afterwards, we designed an experimental setup combining a microscope, laser, fluorescent camera and electromagnet. This setup allowed to carry out the realtime observation of the capsules in a blood stream. The next step was in vitro trapping of the capsules moving in a blood stream through an artificial glass vessel (Figure 1). Finally, we trapped the capsules in vivo in a rat mesentery blood vessel. We found out that the capsules can be effectively stopped by non-uniform magnetic field applied upstream from the injection place (Figure 2). We believe, that this approach is perspective for development of targeted delivery systems and can be promising for further cancer therapy.

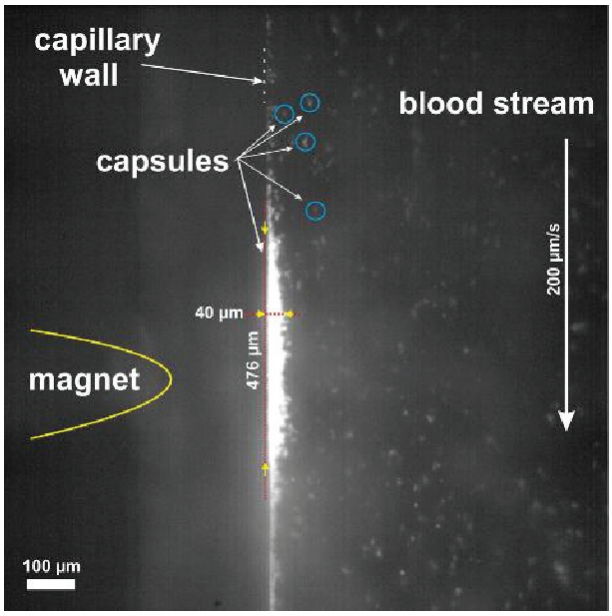


Figure 1. In vitro trapping of fluorescent magnetic microcapsules in a whole blood stream in a glass vessel.

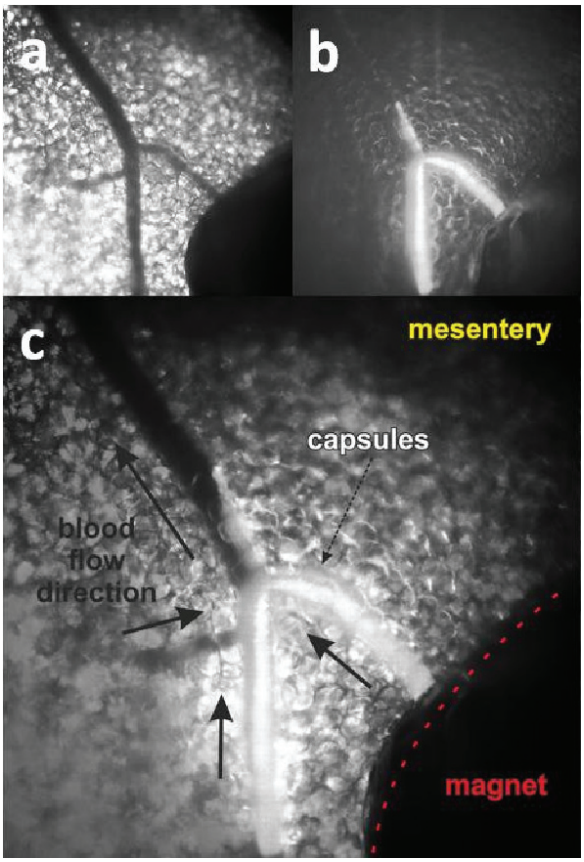


Figure 2. Image of rat mesentery blood vessel in a blue-LED light (1,56 W) before microcapsules injection (a); Fluorescent image of blood vessel with microcapsules trapped by magnetic field. The fluorescence was excited by green 532 nm laser (20 mW) (b); Merged image of the blood vessel with the trapped microcapsules in a blue (LED) and green (laser) light (c).

Zhigilei Leonid
PhD
Professor

Large-scale atomistic simulations of the structural transformations in short pulse laser processing of metals

SCIENTIFIC ORGANIZATION

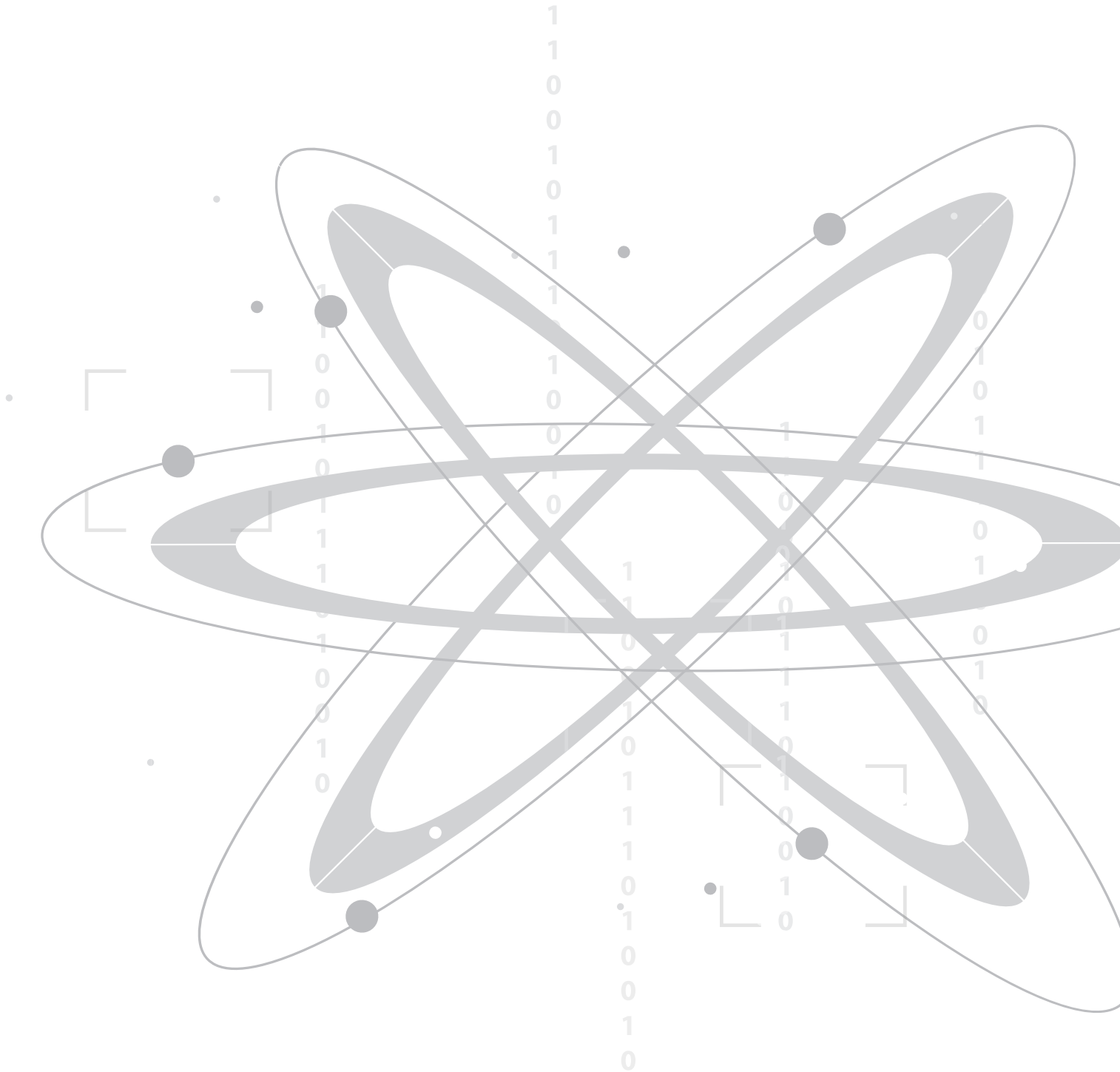
University of Virginia

ABSTRACT

The mechanisms of material ejection and surface modification in short-pulse laser processing of metal targets are investigated in large-scale atomistic simulations performed with a model that combines the classical molecular dynamic method with a continuum description of the laser excitation of conduction band electrons, electron-phonon coupling and electron heat conduction. The results of the simulations reveal a complex picture of highly non-equilibrium processes responsible for material modification and/or ejection in response to the fast laser energy deposition.

KEYWORDS

Laser-materials interactions, molecular dynamics simulations.



PHYSICS & ASTRONOMY

Akimov Dmitry
PhD
Head of laboratory

Experiment on first observation of coherent elastic neutrino-nucleus scattering

SCIENTIFIC ORGANIZATION

Kurchatov Institute

ABSTRACT

The experiment on first observation of the elastic coherent scattering of neutrino off atomic nuclei is proposed with the use of the RED-100 emission two-phase xenon detector. This process was theoretically predicted more than 40 years ago but has not been observed yet. The detector has been build with the help with funding of the mega grant financial support.

KEYWORDS

Neutrino, two-phase emission detector, low-background experiment, neutrino monitoring of nuclear reactor.

SUMMARY

The RED-100 two-phase emission detector has been built in the framework of the mega grant 11.G34.31.0049 for observation of neutrino coherent elastic scattering off atomic nuclei predicted by the Standard model. This process has not been observed yet due to lack of the detection technique of the events with the low energy deposition: the energy of nuclear recoil from the neutrino scattering in detector is in the keV- and sub-keV- energy ranges. The technology of particle detection by means of a two-phase emission detector proposed in Russia and well worked out in the experiments on search for dark matter allows one to perform this. The proposed experiment at the Kalinin nuclear power plant (KNPP) is described in this talk. The perspective of the use of such type detectors for neutrino monitoring of nuclear power reactors is considered.

Arzhannikov Andrei
Doctor of Physics and Mathematics, Professor
Leading scientific researcher

Generation and Application of MM and Sub-MM Radiation

SCIENTIFIC ORGANIZATION

Novosibirsk State University

ABSTRACT

This paper describes results of the modern experimental and theoretical studies on generation of MM and sub-MM waves and their applications. Achievements in scientific research and engineer design for the frequency range from 0.1 up to 1 THz are reviewed. Gyrotrons are the most suitable devices to generate radiation in the frequency area 0.03 – 0.3 THz. For generation in the interval 0.3-1THz a strong interaction of a relativistic electron beam with dense plasma has a good prospect. Applications of such waves have are also analysed in the paper.

KEYWORDS

E-beam interaction with plasma, terahertz radiation, generation and applications of mm and sub-mm waves.

ACKNOWLEDGEMENTS

The research work in LPIMTI NSU was conducted under the Government Decree #220: Contract number № 11.G34. 31.0033. In this time the work is financially supported by RSCF Project #14-12-00610 (EM-wave emission by beam-plasma system) and by the Ministry of Education and Science of RF under the State Assignment Contract #3002 (development of the radiometric system).

SUMMARY

Modern Studies on Generation and Application of MM and Sub-MM Radiation

Andrey Arzhannikov and Manfred Thumm

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This paper describes results of modern experimental and theoretical studies on generation of mm and sub-mm waves and their various applications. Achievements in scientific research and engineering design in the frequency range from 0.1 up to 1 THz are reviewed.

Gyrotrons are the most suitable devices to generate high-power radiation in the frequency region 0.03 – 0.3 THz. Free electron lasers (FEL) are appropriate for the frequency range higher than 1 THz. Nevertheless, to generate very high power pulses in the frequency interval 0.1 -0.5 THz one can use a free electron maser (FEM) with a strongly elongated electron (E)-beam cross section and two-dimensional distributed feedback. To achieve high power radiation in the frequency interval 0.3-1THz, we proposed in 2010 to use the electromagnetic (EM) wave emission from a plasma column due to the process of strong interaction of a relativistic E-beam with the dense plasma.

Studies on mm-wave generation by the FEM with an elongated E-beam cross section and on the EM wave emission from dense plasmas due to plasma interaction were conducted in the Laboratory of Prospective Research on Millimeter and Terahertz Radiation at Novosibirsk State University (LPIMTR NSU) in collaboration with the Budker Institute of Nuclear Physics. Experimental research in this Laboratory at the GOL-3 and GOL-PET devices demonstrated a good prospect of the E-beam-plasma interaction method to generate sub-mm waves with tens MW power.

Millimeter and sub-mm waves have a very wide area of applications in science, industry and usual people life. The activity on investigation of applications of such waves includes the study on plasma heating, current drive and diagnostics in controlled thermonuclear fusion reactors and on the influence of EM-radiation on biological objects, physics methods in medical treatment, industrial production of nano-ceramics, searching of hidden objects by protection systems (e.g. in airports) and mm-wave beams for high resolution radars, wireless power transmission and so on. Such different application areas are also analysed in the paper.

The research work in LPIMTR NSU was conducted under the Government Decree #220: Contract number № 11.G34. 31.0033. Currently, the work is financially supported by RSCF Project #14-12-00610 (EM-wave emission by beam-plasma system) and by the Ministry of Education and Science of RF under the State Assignment Contract #3002 (development of the radiometric system).

Baimuratov Anvar

PhD

Research Fellow

The optical activity of semiconductor nanostructures and nanostructured media

SCIENTIFIC ORGANIZATION

ITMO University

ABSTRACT

We propose and develop an original generic method of engineering optical activity in semiconductor nanocrystals and and nanostructured media, which may prove useful for applications in biology, chemistry, and medicine. The developed theory is illustrated by the example of semiconductor nanocrystals, whose electronic subsystem is perturbed via ion doping or chiral distortion. We also demonstrate that arrangement of achiral nanoobjects in a chiral assembly may result in highly optically active superstructures.

KEYWORDS

Chirality, nanocrystals, circular dichroism, quantum dots.

ACKNOWLEDGEMENTS

This work was funded by Grant 14.B25.31.0002 and Government Assignment No.3.17.2014/K of the Ministry of Education and Science of the Russian Federation. A.S.B. acknowledges the scholarship of the President of the Russian Federation for young scientists. We also acknowledge the financial support from Science Foundation Ireland (Grant SFI 12/IA/1300).

SUMMARY

1. Perturbation of electronic subsystem

We examine the most general case in which there are not degenerate states in the nanocrystal electronic subsystem and all of these states are coupled to each other by the small perturbation. Since some of the transitions between the unperturbed states are electric or magnetic dipole allowed, an arbitrary transition between the perturbed states becomes optically active. In the first order of the perturbation, the rotatory strength of such transition is decomposed on electric dipole and magnetic dipole contributions, which correspond to the electric dipole allowed and magnetic dipole allowed transitions between the quantum states of the unperturbed nanocrystal. The rotatory strengths of these two kinds of transition are of the same order of magnitude, while the dissymmetry factors of the magnetic dipole allowed transitions exceed those of the electric dipole allowed transitions by orders of magnitude. We show that it is possible to achieve the total dissymmetry of the optical absorption upon the magnetic dipole allowed transitions and elucidate the conditions required to do this.

2. Ion doping

We apply the developed theory to describe optical activity of the ion-doped nanocrystals in the form of rectangular parallelepipeds. An impurity ion injected in the crystal lattice perturbs the electronic subsystem of the nanocrystal, which can make the nanocrystal optically active. We analyse the dependence of the rotatory strength on the position of an impurity ion inside a nanocrystal and show that the optical activity of doped nanorods and quantum dots can be 100 times stronger than that of typical chiral molecules.

3. Superstructures

Since chiral nanoparticles are much smaller than the optical wavelength, their enantiomers show little difference in the interaction with circularly polarized light. This scale mismatch makes the enhancement of enantioselectivity in optical excitation of nanoobjects a fundamental challenge in modern nanophotonics. Here we demonstrate that a strong dissymmetry of optical response from achiral nanoobjects can be achieved through their arrangement into chiral optically active superstructures with the length scale comparable to the optical wavelength. This concept is illustrated by the example of the simple helix supercrystal made of semiconductor quantum dots. We show that this supercrystal almost fully absorbs light with one circular polarization and does not absorb the other. The giant circular dichroism of such a supercrystal comes from the formation of chiral bright excitons, which are the optically active collective excitations of the entire supercrystal. Owing to the recent advances in assembly and self-organization of nanocrystals in large superparticle structures, the proposed principle of enantioselectivity enhancement has great potential of benefiting various chiral and analytical methods, which are used in biophysics, chemistry, and pharmaceutical science.

Barannikov Aleksandr
Student
Laboratory assistant

Micro-Optics Test Bench based hard X-ray source

SCIENTIFIC ORGANIZATION

Immanuel Kant Baltic Federal University

ABSTRACT

In 2015, within the implementation of the grant № 14.Y26.31.0002 by the Ministry of Science and Education of the Russian Federation, the optics test bench has been assembled in the Coherent Optics laboratory at the Baltic Federal University. The main goal of the optics test bench is the development and characterization of micro/nano-focusing optical elements. The facility is built as flexible as possible in order to support the characterization of a large variety of optical systems. In addition the optics test bench can be used for the phase contrast imaging and microscopy experiments.

KEYWORDS

Hard X-ray source, liquid anode, micro-optics test bench.

ACKNOWLEDGEMENTS

The results of the project were achieved with support of the Ministry of Education and Science of the Russian Federation as a part of the agreement № 14.Y26.31.0002 under the program to attract scientists in the Russia with a worldwide reputation for creating a competitive research laboratories launched by the Russian Federation Government Decree № 220.

SUMMARY

In 2015, within the implementation of the grant № 14.Y26.31.0002 by the Ministry of Science and Education of the Russian Federation, the optics test bench has been assembled in the Coherent Optics laboratory at the Baltic Federal University. The main goal of the optics test bench is the development and characterization of micro/nano-focusing optical elements. The facility is built as flexible as possible in order to support the characterization of a large variety of optical systems including refractive lenses, Bragg- Fresnel lenses, Fresnel zone plates, reflective optics based either on mirrors or multilayers, focusing crystals, capillaries and waveguides. In addition the optics test bench can be used for the phase contrast imaging and microscopy experiments.The optics test bench consists of the microfocus “Metal Jet” X-ray tube with liquid Ga anode, optics, diagnostics or sample and detector stages. The main activities within this setup are tests of compound refractive lenses made from Al, Be and diamond materials in terms of efficiency and focusing. The most recent optics test bench project is an X-ray microscopy based on 161 epoxy spherical concave individual lenses with the radius of curvature of 50 μm. We hope that the test bench will produce more extraordinary results in the field of x-ray micro-/nano-optics, microscopy and imaging techniques that can directly contribute to the high quality of research.

ADDITIONAL INFORMATION

Application for the grant of a Russian patent Test bench for refractive X-ray optics” Authors: A.Goikhman, P. Prokopovich, A. Borisov, I.Panormov, N. Klimova, P.Ershov , D.Serebrennikov, D.Zverev, A.Barannikov, Applicant: FGAOU VO “BFU Immanuel Kant.” Reg. Number 2015155999 from 12.25.2015. The continued examination of the merits.

Bart Verberck
PhD
Senior Editor, Nature Physics

Publishing and Nature Research Journals

SCIENTIFIC ORGANIZATION

Springer Nature

KEYWORDS

Publishing, Springer Nature, Nature Physics, Science Communication.

SUMMARY

Publishing plays an important role in science. In the 21st century, publishers' roles and services have evolved enormously. In this presentation, I will introduce Springer Nature, the result of a recent merger between Nature Publishing Group, Palgrave Macmillan, Macmillan Education and Springer Science+Business Media. I will reflect on some of the activities of Springer Nature in general, and on publishing in Nature Research Journals in particular. The main aim of the presentation is to show how publishers are much more than a platform for publishing scientific results — how they can cater for the needs of scientists, today and in the future. I will also discuss my role as a Nature Physics editor and explain the editorial process at Nature Research Journals, including criteria for publication. Finally, I will use the opportunity to provide some advice on scientific writing and communicating research.

Baturin Vladimir
PhD
Research fellow

Lepeshkin Sergey
PhD
Research fellow

Structure and stability of silicon-oxide nanoclusters: the formation of reactive oxygen species on the surface

SCIENTIFIC ORGANIZATION

Moscow Institute of Physics and Technology

ABSTRACT

Oxidation of silicon nanoclusters going through all oxygen concentrations is explored from first principles using the evolutionary algorithm, structural and thermodynamic analysis. The most involved processes take place at the cluster surface, where 12 characteristic groups of Si-O atoms, many of which are magnetic and relevant to reactive oxygen species (ROS), are distinguished. Our thermodynamic analysis provides p-T conditions at which clusters with different oxidation exist. These results are useful for miscellaneous applications, including biomedical ones.

KEYWORDS

Ab initio calculations, nanomaterials, structure prediction.

SUMMARY

Oxidation of silicon nanoclusters going through all oxygen concentrations is explored from first principles using the evolutionary algorithm, structural and thermodynamic analysis. Calculations are performed for 90 clusters SinOm with $n \leq 10$ and $m \leq 2n+9$. Considering the Si7Om clusters with $0 \leq m \leq 23$ as a model system, we analyze changes in their structure and energetics. The most involved processes take place at the cluster surface, where 12 characteristic groups of Si-O atoms (CGA), many of which are magnetic and relevant to reactive oxygen species (ROS), are distinguished. In all clusters oxidation shows itself as the consecutively appearing CGAs, which follow in the order dictated by their energetics and geometry. Thermodynamic analysis reveals clusters with ROS existing at the ambient conditions that rises biomedical issues.

ADDITIONAL INFORMATION

Sergey Lepeshkin (co-author)

Bayer Manfred
Prof. Dr.
Full professor

Spin physics in the XXIst century: Joining forces of megagrants in an international collaborative research center

SCIENTIFIC ORGANIZATION

TU Dortmund University

ABSTRACT

The spins of electrons and nuclei are exploited intensely in today's technological applications such as nuclear magnetic resonance or information storage. However, it is common believe that spins offer much more appealing functionalities, in particular when exploiting their quantum mechanical properties. In this contribution I will give a couple of examples for novel strategies by which spins may be controlled and manipulated in a coherent, energy-efficient way so that they may form the basic building blocks for future information technologies.

KEYWORDS

Spin, lasers, optics.

ACKNOWLEDGEMENTS

This work is supported by the Russian Ministry of Education and Sciences (contracts no. 14.Z50.31.0021 with M. Bayer as leading scientist and 11.G34.31.006 with A. Kavokin as leading scientist). Also the support in the frame of the International Collaborative Research Center TRR 160, "Coherent manipulation of interacting spin excitations in tailored semiconductors", by the Russian Foundation of Basic Research and the Deutsche Forschungsgemeinschaft is acknowledged.

SUMMARY

This contribution describes the research efforts pursued since a couple of years in a complementary way in the frame of two megagrants located at St. Petersburg: the Hybrid Spinoptronics Laboratory at the Ioffe-institute and the Spin Optics Laboratory at the St. Petersburg State University. Both have provided the decisive infrastructure for performing research on novel spin-based hardware which may form the basis for a new area of information technology. The activities comprise efforts in developing tailored hardware for spin excitations with long lifetime, implementing controlled interactions between spins, developing techniques for controlling spins by optimized laser and microwave pulses as well as inventing designs for optimal manipulation strategies. A central goal is to perform spin manipulation such that the required energy for each operation is minimized. In that way the technology would become particularly energy-efficient, while simultaneously offering fast and superior operation - a more and more important demand nowadays, as the energy consumption in information technologies is continuously increasing. Ultimately it may be possible to combine all components required for information processing, processors and memories, into a single chip, allowing further device miniaturization and increase of performance. Also the extension from classical information technology into the quantum regime is explored. By exploiting coherent quantum superposition states of spins, which resemble implementations of the famous Schroedinger's cat, it may be possible to provide essential contributions to the areas of inherently secure quantum communication or quantum computing, in which problems can be solved with unprecedented speed.

Within this initiative several promising candidate systems are explored such as semiconductor-ferromagnet hybrids, combinations of plasmonic and semiconducting structures or polariton condensates, which are studied by innovative spectroscopies that are developed and adapted for these systems. The experimental efforts are accompanied by detailed theoretical calculations. The activities have turned out to be so successful that both MegaGrants have joined forces in an International Collaborative Research Center titled "Coherent manipulation of interacting spin excitations in tailored semiconductors" funded by the Russian Foundation of Basic Research and the Deutsche Forschungsgemeinschaft, which is operating since beginning 2015. Being the first initiative of this kind and size between Russia and Germany, this research center will be presented with respect

to its mission that in particular includes training of a new generation of scientific leaders in the field. This target shall be achieved by an intense exchange of PhD students and postdoctorial researchers between St. Petersburg and Dortmund. The exchange will be the basis for obtaining a sustainable leading position of the initiative in the international research community. This ambition will be underlined by presenting the first results obtained in the research center, published in leading scientific journals.

Belosludov Vladimir
Professor
Leading senior researcher

Theoretical Study on Clathrate Hydrate for Energy Storage and Transport

SCIENTIFIC ORGANIZATION

Nikolaev Institute of Inorganic Chemistry, SB RAS

ABSTRACT

Our main target for gas storage materials is clathrate hydrate, which is expected to be the cleanest energy carrier, since it stores various gas molecules. We have applied our theoretical methods described above and studied a number of cases to stabilize clathrates hydrate with help gas for efficient hydrogen storage to be able to be used industrially; such as hydrogen car. We apply thermodynamics to estimate P-T phase diagram to serve important information for practical usages. We now can predict higher density gas storage materials with theoretical confidence prior to experiment.

KEYWORDS

Clathrate hydrat, thermodynamics, P-T phase diagram, hydrogen storage, energy carrier.

ACKNOWLEDGEMENTS

The author is thankful to the Russian Megagrant Project No.14.B25.31.0030 “New energy technologies and energy carriers” for supporting the present research.

SUMMARY

- Formalism for calculating the thermodynamic properties of a clathrate hydrate with weak guest-host interactions was realized. The proposed model accounted for multiple cage occupancy, host lattice relaxation, and the description of the quantum nature of guest behavior [1]:using this approach, the phase diagrams of the pure and binary hydrogen hydrates were constructed and they are in agreement with available experimental data [2-7]. In order to evaluate the parameters of weak interactions, a time-dependent density-functional formalism and local density technique entirely in real space have been implemented for calculations of vdW dispersion coefficients for atoms within the all-electron mixed-basis approach. The combination of both methods enables one to calculate thermodynamic properties of clathrate hydrates without resorting to any empirical parameter fittings [8]. Using proposed approach, the phase diagrams of various clathrate hydrates and obtained results are in agreement with available experimental data;
- it has been found that the pure hydrogen cubic structure II (CS-II) hydrate is more thermodynamically stable than the cubic structure I (CS-I) hydrate in a wide range of p–T regions. However, at low pressure, the stabilization of the CS-I hydrate can be realized for H_2–C_2H_6–H_2O systems even with small concentrations of ethane in the gas phase. However, in this case, the amount of stored hydrogen strongly depends on the ethane concentrations in the gas phase. At low concentration of ethane, the amount of hydrogen stored, 2.5 wt%, in CS-I hydrate can be achieved at T = 250K. We believe that the present approach can be useful for understanding the thermodynamic properties of the binary hydrate and it can support the experimental exploration of novel hydrogen storage materials based on clathrate hydrates;
- it has been found that at a small methane concentration in the gas phase the stable hydrate phase has cubic structure II (CS-II) and at a methane concentration

of 6% stabilizes cubic structure I, which is metastable in the case of the pure hydrogen hydrate. This is in agreement with recent experimental data. The amount of hydrogen storage depends on the methane concentration in the gas phase as well as the thermodynamic conditions of hydrate formation. Hydrogen storage up to 2.6 wt.% can be achieved in the binary H_2-CH_4 CS-II hydrate at T=250 K. Despite the fact that these conditions do not satisfy the criteria for onboard hydrogen storage applications, the present binary clathrate hydrate can be considered as a promising candidate for the large-scale stationary storage in urban areas or industrial complexes. In contrast to large molecules such as *tetrahydrofuran (THF)* or propane, the stabilization of the CS-II hydrate is forced by occupation of both the small and large cages. Therefore, four fold hydrogen occupancy can be easily achieved due to the low ratio of occupied large cavities;

- theoretical modeling of argon + hydrogen mixed hydrate phase diagram and hydrate composition has been performed. For this purpose the original approach allows to take into account multiple cage occupancy with possibility of mixed clusters as well as influence of guest molecules on the host lattice has been used. Separately, argon and hydrogen form CS-II hydrates. We considered only CS-II gas hydrates formation. It is shown that thermodynamic stability of mixed argon + hydrogen hydrates strongly depends on presence of argon in the gas phase as the heavier component. Thus, with increasing argon content in the system, hydrate stability field extends to low pressures with increasing argon fraction in the small cavities. Furthermore, we observed no mixed occupation of the large hydrate cavities by Ar + H_2 clusters. It has been shown that the addition of argon, as a heavier component in the gas mixture, reduces the pressure of hydrate formation, however, this causes a decrease in hydrogen content in the hydrate. It is estimated that for large cavities of hydrate filling by clusters of four hydrogen molecules is preferable. Small cavities are more suitable for filling with argon atoms;
- thermodynamic properties hydrogen clathrate hydrates (CS-II) and ice I_h and pressure of clathrate hydrate phases immersed in the ice I_h phases have been investigated using both lattice dynamics and molecular dynamics methods with the aim to understand the existence of self-preservation effect in hydrogen hydrate in the framework of molecular–level models;
- the statistical thermodynamics model with some modifications describing host lattice relaxation, guest-guest interactions and the quantum nature of guest behavior in clathrate hydrates was applied to calculate the relative thermal expansion, i.e. ratio of volume at temperature T and pressure P_0 to volume at T_0, P_0, of hydrogen clathrate hydrate as well as for ices. As reference points the temperature and pressure were selected as T_0 = 140 K and P_0 = 0.1 MPa, respectively. It was shown that hydrate phases immersed in the ice phases are stable below the three-phase ice–hydrate–gas equilibrium pressure. The hydrate phase remains thermodynamically stable under heating. The calculations show that the pressure in the hydrogen clathrate hydrate sphere immersed into the ice matrix is notably higher than the pressure inside the ice phase, but it does not lead to system distortion because of the formation of a network of hydrogen bonds between hydrate and ice phases. This is because the thermal expansion of hydrogen hydrate is larger than that of ice. Hydrate can be stay in region of its stability on phase diagram because thermal expansion of hydrate phase limited by thermal expansion of ice. Such difference of thermal expansion should lead to self-preservation effect by appearing additional pressure. From a practical point of view this effect can be used for storage and transport of hydrogen in the hydrate form [9].

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Observables sensitive to tensor structure of di-photon interaction of a hypothetical heavy spin-0 boson

SCIENTIFIC ORGANIZATION

National Research Nuclear University MEPhI

ABSTRACT

We study observables sensitive to tensor structure of interactions of a hypothetical heavy spin-0 boson. It is assumed that interactions of this particle are dominated by interactions with photons. The above assumptions favor the production of this hypothetical particle through the VBF mechanism structurally dominated by the photon and Z-interactions. This particle will be produced in association with two light quarks. It is shown that the azimuthal angle difference between the tagging jets provides an observable to probe the tensor structure of the interaction vertices.

KEYWORDS

BSM, Heavy particle, Tensor structure, Extended Higgs sector, photon, jets, VBF, CP.

ACKNOWLEDGEMENTS

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ADDITIONAL INFORMATION

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Advances in Silicon Photomultiplier development and applications

SCIENTIFIC ORGANIZATION

Moscow engineering physics institute

ABSTRACT

We report on our group's recent progress in the development of silicon photomultipliers (SiPM), and their applications in both particle and astroparticle physics, including (but not limited to) medical physics applications (neutron therapy), the Belle-II particle physics experiment in Tsukuba, Japan, the ANITA/HiCal astroparticle physics experiment in Antarctica, and the planned Intenational Linear Collider (ILC) experiment.

KEYWORDS

Silicon Photomultipliers, particle physics, astroparticle physics, medical physics.

ACKNOWLEDGEMENTS

This work is supported by the Russian Ministry of Education and Science contracts 14.A12.31.0006 and 4465.2014.2 and the Russian Foundation for Basic Research grant 14-02-01220. We are also grateful for the support of our host institution (Moscow Engineering Physics Institute).

SUMMARY

1) Silicon photomultipliers are particularly promising as sub-atomic particles, owing to their robustness (insensitivity to external magnetic fields, in constrast to conventional high-voltage photomultiplier tubes), their ability to be operated at relatively modest bias voltages, their compact size, and their ability to render tens-of-micron scale positional resolutions.

2) Our work has focused on understanding the atomic-level characteristics of silicon photomultiplier signal development in order to refine and optimize our range of applications.

3) Internationally, our group has led the development of silicon photomultiplier detectors for the Belle-II particle physics experiment in Tsukuba, Japan, currently being commissioned, as well as the ANITA-HiCal experiment in Antarctica, which is being prepared for launch in December, 2016.

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Advances in Silicon Photomultiplier development and applications

SCIENTIFIC ORGANIZATION

Moscow engineering physics institute

ABSTRACT

We report on our group's recent progress in the development of silicon photomultipliers (SiPM), and their applications in both particle and astroparticle physics, including (but not limited to) medical physics applications (neutron therapy), the Belle-II particle physics experiment in Tsukuba, Japan, the ANITA/HiCal astroparticle physics experiment in Antarctica, and the planned Intenational Linear Collider (ILC) experiment.

KEYWORDS

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SUMMARY

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SCIENTIFIC ORGANIZATION

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Thin-film photoconductive antennas using low-temperature GaAs grown on a GaAs substrate of different crystallographic orientation for the generation and detection of terahertz waves

ABSTRACT

Our work is devoted to investigation of photoconductive antennas with delta-doped layers of low temperature LT-GaAs, grown by molecular beam epitaxy at a temperature of 230 °C on GaAs substrates with the crystallographic orientation of 100 and 111. The method of “pump-probe” THz spectra were obtained with a peak resonance frequency of 0.96 THz. It has been found that the efficiency of generating the THz radiation in the antenna field applied to 111 GaAs substrate is much higher in comparison with the 100 substrate.

KEYWORDS

LT-GaAs, Photoconductive antennas, Terahertz generation.

ACKNOWLEDGEMENTS

The Ministry of Education and Science of the Russian Federation (Grant No. 14.Z50.31.0034) supported this work.

SUMMARY

Photoconductive semiconductor structures based on low-temperature LT-GaAs with planar dipole antennas are the most common devices for the generation and detection of terahertz radiation [1]. Multilayer structures LT-GaAs (low-temperature grown GaAs, the low-temperature “of gallium arsenide) are studied, for the modern high-speed communication applications, for example, in ultrafast optical network switches [2]. The creation of such switches will dramatically increase the speed of data transfer. In addition, this material is used for the rapid and sensitive photodetectors. [3]

The study was made using the optical “pump-probe” technique. As the irradiation source the TiSa laser with the wavelength of 800nm was used (photon energy of 1.55 eV), and a pulse duration of 100 fs. The pump pulses passes through a delay line oscillator and focused on the surface generated THz radiation. Further, THz radiation was collect by parabolic mirrors and focused on non-linear ZnTe crystal. On the ZnTe crystal THz sensing and came down. The principle of operation is based on the interaction of terahertz and optical radiation in a nonlinear medium. Due to the non-linearity the optical signal (high frequency) was modulated by terahertz irradiation (low frequency).

The results of THz spectra generated by antennas based on LT-GaAs with different type of substrate are shown in Table 1. It is seen that the efficiency of the antenna on a GaAs substrate 111 section crystallographic 2-fold higher. Most likely, this is due to the high concentration of free electrons in the 111 structure. The electric field accelerate the free charges on the surface and emit in a broad band corresponding to the terahertz frequency range. Spectral width depending on the slice has not changed. The narrow spectrum of THz radiation is most likely associated with limiting the possibility of detecting non-linear ZnTe crystal.

Antenna Type (Crystallographic section)	The efficiency of THz radiation (au. un.).	Bandwidth
(THz)		
100	5,98	2,79
111	12,23	2,79

Thus, it is shown that the efficiency of the antenna TGts- based on LT-GaAs formed on the substrate 111 with the crystallographic section of 2 times more effective than a similar structure made on the substrate 100 with the crystallographic section.

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The temperature dependence of Sn2P2S6 crystal nonlinear optical response study by the time-resolution spectroscopy technique

SCIENTIFIC ORGANIZATION

Moscow Technological University (MIREA)

KEYWORDS

Second harmonic generation, ferroelectric- semiconductor, time-resolution spectroscopy.

ACKNOWLEDGEMENTS

This work is supported by Russian Ministry of Science and Education (contract № 14.Z50.31.0034).

SUMMARY

One of the main problem of modern micro - and nanoelectronics is the searching for new materials for creation of new generation of multifunctional electronic components, as well as a comprehensive study of the functional and structural properties of these materials.

Various magnetic materials and structures are traditional objects of research in this area. The fastest way to switch magnetic moment is the impact of ultrafast electromagnetic pulses, for example, femtosecond laser pulses.

Ferroelectric materials are an alternative of magnetic materials to create nonvolatile memory. For example, the optical polarization switching can be realized in ferroelectric-semiconductors due to the influence of the electron subsystem on the ferroelectric and electrical characteristics.

The material $Sn_2P_2S_6$ was chosen to investigate this possibility, because it is a ferroelectric- semiconductor by nature, and the potential of its use as electronic components is higher than that of ordinary ferroelectrics.

For a new generation of electronic devices high-speed processing and storage of information the possibility of optical control using femtosecond laser pulses of the polarization state of coherent quantum control of phonons is expected.

In this work we present the experimental study results of the nonlinear optical response temperature dependence in ferroelectric-semiconductor $Sn_2P_2S_6$ (SPS) near the phase transition temperature. The dynamics of the nonlinear optical response relaxation in $Sn_2P_2S_6$ crystal was studied by the time-resolution spectroscopy technique in the picosecond time range. In this experiment, the crystal temperature was passing through the phase transition temperature.

The absence of Curie temperature effective change in the crystal under the femtosecond laser radiation action was shown, as well as the low threshold of material destruction were made.

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The TAIGA experiment: from cosmic ray to gamma-ray astronomy in the Tunka valley

SCIENTIFIC ORGANIZATION
Irkutsk State University

ABSTRACT

The physical motivations and advantages of the new gamma-observatory TAIGA (Tunka Advanced Instrument for cosmic ray physics and Gamma Astronomy) is presented. The TAIGA array is a complex, hybrid detector for ground-based gamma-ray astronomy for energies from a few TeV to several PeV as well as for cosmic ray studies from 100 TeV to several EeV. The recent results of measurements including first observation of very high energy gamma ray of the Crab nebula with first cluster of wide angle Cherenkov array TAIGA-HiSCORE are presented.

KEYWORDS

High energy gamma-astronomy, cosmic ray physics, gamma-observatory TAIGA, Crab nebula.

ACKNOWLEDGEMENTS

This work was supported by the Russian Federation Ministry of Education and Science (agreement 14.B25.31.0010), the Russian Science Foundation (grant 15-12-20022) and by the Russian Foundation for Basic Research (grants 15-02-05769 and 16-02-00738).

SUMMARY

In recent years gamma-ray astronomy became the most dynamically developing field of astroparticle physics. More than 150 sources of TeV gamma – ray were discovered and studied. However, until now there was not detected a single photon with energy above 80 TeV. Essentially, this is explained due to the fact that the most of formerly and currently existing arrays are a network of Imaging Atmospheric Cherenkov Telescopes (IACT): HEGRA, H.E.S.S., MAGIC and VERITAS with the level of sensitivity optimized for the energy range 100 GeV - 20 TeV. Although, there are a lot of fundamental questions without answers about processes in the range of high and ultra-high energies. The so-called 4th generation IACT array CTA as well HAWC and LHAASO will have substantially higher sensitivity than the existing telescopes in the energy range of up to 100 TeV, but not sufficient to solve all problems of very high energy gamma – astronomy.

To solve many crucial tasks of high energy gamma-astronomy as well cosmic ray physics we propose to design and to construct the gamma-observatory TAIGA (Tunka Advanced Instrument for cosmic ray physics and Gamma Astronomy) - a complex hybrid detector system including: wide-angle Cherenkov detectors, IACTs, electron, muon and radio detectors grouped into 6 arrays. Common operation of an array of IACTs and a wide-angle Cherenkov array can allow one to abstain from simultaneous measurement of the EAS in stereoscopic mode by several closely packed IACT and thus allows to increase the distance between IACT up to

600 -1000 m reducing the number of telescopes needed by a factor of four times or more. In the combination of both techniques, the timing array provides the information about shower core position, incidence angle and energy, and the IACT images are used for the identification of the primary particle.

TAIGA will be located in the Tunka valley, about 50 km from Lake Baikal in Siberia, Russia, were since 2009 the full-size Tunka-133 Cherenkov EAS detector is in operation. The experience of Tunka-133 on the energy spectrum and mass composition of cosmic rays, together with it's existing infrastructure are important factors for selecting this location. TAIGA will combine six arrays with different types of detectors.

TAIGA will combine six arrays with different types of detectors.

1. The Tunka-133 array. The Tunka-133 array consists of 175 wide-angle Cherenkov detectors distributed over 3 km2 area. The detectors are grouped into 25 clusters, each with 7 detectors—six hexagonally arranged detectors and one in the center. The distance between the detectors in each cluster is 85 m. The energy spectrum and mass composition of cosmic rays in the range of 6–1000 PeV has been reconstructed using data from 5 winter seasons of measurements with the Tunka-133 array. The spectrum has a rather complicated structure with different power-law index and points out reliably the existence of a "second knee" at 300 PeV, probably, it is manifestation of a transition from galactic to extragalactic origin of the cosmic rays. We find a decrease of the mean (in logarithm) of the atomic number or composition, this lightening at energies higher than 100 PeV also points to a transition to extragalactic cosmic rays.

2. The TAIGA-HiSCORE array. The principle of the TAIGA-HiSCORE array is rather similar to the one used for the Tunka-133 array. Again, this method is based on the sampling of the Cherenkov light front of air showers. The TAIGA-HiSCORE will consist of an array of 500 wide-angle (field of view 0,6sr) light-sensitive detector stations, distributed with spacing 75 – 200 m over an area of a five square kilometer, probably the array area will be extended in future. The array threshold for gamma-ray induced EAS is 30 TeV, for cosmic rays 100 TeV. The TAIGA –HiSCORE data allow to reconstruct the arrival direction of the EAS with an accuracy of about 0.1 degree, the core location to 5–6 m, energy to 10-15% and shower maximum height Xmax 20 – 25 g/cm^{2}.

3. The TAIGA- IACT array will include 16 Imaging Atmospheric Cherenkov Telescopes distributed with 600 – 1000 m spacing over an area of 5 km2. Each HEGRA-like telescope of the array will be composed of a mosaic, 34-segment reflector in Davis-Cotton design, with a diameter of individual mirrors 60 cm. The full diameter of the reflector is 4.3 m, the area ~10 m2, the focal length 4.75 m. The Imaging camera consist of 547 photomultipliers and will have a field of view (FOV) of 9,72 x 9,72 degrees and an angular size of 0.36 degrees per pixel. The IACT array energy threshold for gamma-rays is 1 TeV, the sensitivity in the energy range 1-20 TeV is 10^{-12} erg cm^{-2} s^{-1} for 50 hours of observation with angular of resolution 0.03 degree. The reconstruction of core position, arrival direction and energy of coincident EAS events by the TAIGA-HiSCORE array will help the IACTs to reject the high energy background events on large impact parameters of up to 600 - 1000m. Joint operation of the first Cherenkov telescopes of the TAIGA-IACT and the TAIGA-HiSCORE arrays in the energy range 30-200 TeV will yield a sensitivity of the order of 10-13 erg cm^{-2} s^{-1} (for 10 events in 500 hours of observation) and suppress the cosmic ray background by 50 – 100 times even for IACT spacing of 1000 m.

4. TAIGA Muon and Tunka-Grande: the nets of particle detectors. There are a lot of reasons to include the particle detectors into the hybrid detector complex of the gamma-observatory TAIGA. In particular, the number of muons in a charged cosmic-ray induced EAS is on average 30 times higher than in gamma-ray events, so measuring of muon number is very effective way to suppress background. This should work well for the energy range above 100 TeV. The overall area of muon detectors Sμ should be 0.2-0.3% of the total area of TAIGA-HiSCORE, so we intend to construct a TAIGA-Muon array with an area 2000-3000 m^2. As a first step to future large array to detect EAS electrons and muons we constructed the Tunka-Grande array consisting of 19 scintillation stations, each of them with a surface and an underground part. The stations are located at distances about 20 m from the centres of the Tunka-133 clusters. In November 2015 the deployment of Tunka-Grande was completed and the array was put in operation. Each surface detector includes 12 scintillation counters with a size 80x80 cm^2 formerly operated as part of the EAS-TOP and the KASCADE-Grande

arrays. There are 8 of the same type counters in underground muon detectors. The simulation results show that for energies > 100 PeV Tunka-Grande allows to reconstruct the EAS electron number to 10% precision, muon number - 25%, the EAS arrival direction to about 1.4 degree accuracy, the core location - 17 m, energy - 20%.

5. The Tunka-Rex array is the radio array of the TAIGA observatory. At present time Tunka-Rex consists of 64 radio detectors. They cover area 3 km^2 and are located at distance 20 m about from Tunka-133 cluster centers and scintillation detectors of Tunka-Grande mainly with spacing 200 m. Upon a coincidence trigger of the Cherenkov or the scintillation detectors, both the radio and the air-Cherenkov or scintillation detector are read out in parallel. The electromagnetic field of the radio signal measured by Tunka-Rex is reconstructed in an effective bandwidth of 35 – 76MHz The Tunka-Rex energy precision seems to be at least as good as the published Tunka-133 resolution of 15%. The Xmax precision of Tunka-Rex is roughly 40 g/cm2, and can be slightly increased

In 2016, the TAIGA collaboration has continued the construction of a complex of arrays with hybrid detector systems in order to search for new local Galactic sources of gamma rays with energies higher than 20-30 TeV. We will also study signals from the nearby extragalactic sources Mrk421 and Mrk-501 in order to investigate the gamma-ray absorption on intergalactic background radiation and to search for axion-photon transitions. The study of gamma radiation in the high energy range is of interest not only for astrophysics, but also for testing theories predicting a violation of Lorenz invariance and to search for super-heavy dark matter. Joint operation of the first Cherenkov telescopes of the TAIGA-IACT and the TAIGA-HiSCORE arrays in the energy range 30-100 TeV will yield a sensitivity of order 10-13 erg cm-2^{ 1} s^{-1} (for a 5σ-detection in 500 hours of observation). This sensitivity would allow to measure the energy spectrum of gamma rays from the Tycho SNRs, a main PeVatron candidate. For TAIGA, placed at 53° N/L, this source may be observed during more than 200 hours per year, taking into account 50% of good weather condition. This sensitivity level would allow us to search for signals from the sources observed by IceCube as neutrinos, if these are of Galactic origin, and would allow to make a survey for new PeVatrons

The recent results of measurements including first observation of very high energy gamma ray of the Crab nebula with first cluster of wide angle Cherenkov array TAIGA-HiSCORE are presented.

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Ultrafast processes in the semiconductors based on LT-GaAs doped by delta-layer of Si

SCIENTIFIC ORGANIZATION

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KEYWORDS

Optical spectroscopy, ultrafast, carriers, pump-probe, carried, femtosecond laser.

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SUMMARY

GaAs grown by molecular beam epitaxy at low temperatures (LT-GaAs) appear one of the most perspective materials in the field of ultrafast optical communications. Its use in ultrafast optical commutators [1] will greatly speed up the data transfer, since the charge carriers in this material have greater mobility and shorter lifetime, in contrast to a simple structure based on gallium arsenide [2]. Also, this material is going to be used as a basis for terahertz antennas [2]. Such antennas are used in medicine, which will pass away to replace the X-rays as a terahertz safer.

To investigate the dynamics of charge carriers ultrafast optical spectroscopy technique of “pump-probe” is used. This technique is based on separation an ultrashort

laser pulse into two: the weaker – the probe impulse, stronger - the pump pulse. These two pulses are retained in a special way in relation to each other by a delay line. As a source of laser radiation the tunable femtosecond Ti:sapphire laser with 800nm wavelength and pulse duration 100fs is used. The changes in the reflectance of the probe pulse as a function of time delay between the pump pulse and the probe are detected.

As the test samples was used LT-GaAs growth after annealing. Two types of samples were investigated: with delta doped silicon layer and without it. The samples was grown by molecular beam epitaxy methodic at relatively low temperature (300-400°C) on the (100) GaAs substrate. The width of the bandgap of GaAs in the amount is Eg≈1.4 eV [4].

Typical time dependencies were obtained for B_1 and B_2 structures on the intensity (figure 1). Figure 1 shows that after excitation of semiconductors by photon with 1.5 eV greatly increases the concentration of charge carriers by generating and then there is their recombination.

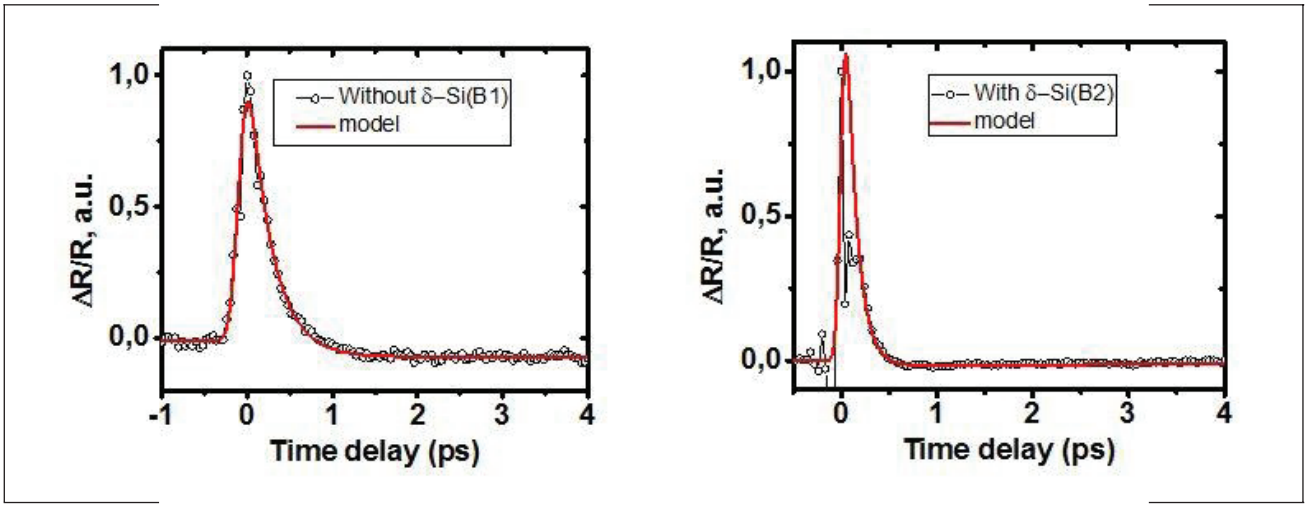

Figure 1. Dependencies of intensity refractive coefficient of probe pulse on the delay time between pulses for the sample Solid line is approximation within the model.

For quantitative analysis of observed approximation process was carried out on an example of the experimental data, previously developed to describe similar processes in direct-gap semiconductors [5-7].

The obtained relaxation times are shown in Table. Typically relaxation time τ_1 for the B_1 and B_2 structures of the same order. However, for the B_1 τ_2 much more than B_2. The same behavior of the relaxation time may be due to the fact that the concentration of defects in LT-GaAs after annealing is decreased, and the delta-doping of silicon creates reduces the lifetime of minority carriers [8,9].

Table 2. Relaxation times

Material number	B_1	B_2
τ_1, ps	0.27	0,11
τ_2, ps	>>100	7,12

Thus, the investigation of LT-GaAs semiconductors with the «pump-probe» femtosecond laser spectroscopy methodic was obtained. During the experiment, the surface of the sample when excited by femtosecond pulses were obtained depending on the response signals from time to time. Approximation of the characteristic relaxation times was obtained. It was shown that the delta-doping silicon layers reduces the lifetime of holes. This behavior is most likely due to a decrease in the concentration of acceptor levels in the structure, with a high donor concentration [9].

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Fine structure of the Mn acceptor in GaAs in external deformation and magnetic field

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ABSTRACT

We determine the electronic level structure of the Mn acceptor in bulk GaAs in presence of applied uniaxial stress and an external magnetic fi eld. Resonant spin-flip Raman scattering is used to measure the g factor of the A0Mn center in the ground and excited states and characterize the optical selection rules of the spin-flip transitions between these states. We determine the random stress fi elds near the Mn acceptor, the constant of the antiferromagnetic exchange interaction and the deformation potential for the exchange energy.

KEYWORDS

Nanostructures, diluted magnetic semiconductors, raman scattering, magneto-optics.

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SUMMARY

We determine the electronic level structure of the Mn acceptor A^0_{Mn} in bulk GaAs in dependence on uniaxial stress and an external magnetic field. Different spectroscopic methods show that the presence of Mn^{2+} impurity leads to the formation of a complex of the valence-band hole bound to a Mn^{2+} ion and that the coupling between the hole and Mn spins is antiferromagnetic. This antiferromagnetic exchange leads to the formation of four levels that are described by the quantum number F = J + S = 1; 2; 3; 4 [1].

Resonant spin-flip Raman scattering is used to measure the g factor of the A^0_{Mn} center in the ground and excited states with the total angular momenta F = 1 and F = 2 and characterize the optical selection rules of the spin-flip transitions between these Mn-acceptor states.

We demonstrate that even without external stress the Mn acceptor experiences random local stress that induces a splitting of the ground F = 1 state of up to 0.7 meV. We determine the random stress fields near the Mn acceptor and the constant of the antiferromagnetic exchange interaction between the valence-band holes and the electrons of the inner Mn2+ shell. It is also shown that uniaxial compressive stress leads surprisingly to a significant reduction of the p-d exchange interaction strength and to a deformation potential value of the exchange constant given by A_p = 0.9 eV. Furthermore, the measured effective g factor of the excited F = 2 states is comparable with the theoretically predicted g = 23/12 value. The developed theoretical model of the Mn acceptor, which considers random local and external uniaxial stresses as well as a magnetic field, satisfactorily describes the observed spin-flip Raman lines and their polarization characteristics. This model highlights that the previously reported value Δ_{F1-F2} of the hole-Mn-ion exchange energy was underestimated by about 20%. By combining the experimental Raman study with the developed theoretical model on the scattering efficiency the fine structure of the Mn acceptor for the multiplets with the total angular momenta F = 1 and F = 2 is determined in full detail.

Our study on the spin-flip Raman scattering of the Mn acceptors in GaAs underlines that their individual properties are essential to explain the stress dependence of the antiferromagnetic hole-Mn exchange interaction. These results may be considered as a step toward understanding the magnetic anisotropy of (Ga,Mn)As as a result of the individual Mn acceptors and may be employed for other acceptor complexes in III-V semiconductor structures.

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Additional information

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Applications of Artificial Intellegence in Crystal Structure Prediction

SCIENTIFIC ORGANIZATION

Moscow Institute of Physics and Technology

ABSTRACT

We present s new method for a fast, unbiased and accurate representation of interatomic interactions. It is a combination of a neural network and our new approach for pair potential reconstruction. The potential reconstruction method is simple and computationally cheap and gives rich information about interactions in crystals. In addition, we present a way on how to analyse features that are included for the description of crystal structures. It helpes to find the most important features and as a result it helps to build physically more relevant model.

KEYWORDS

Neural networks, global search, USPEX, crystallography.

SUMMARY

1. We present our method of potential reconstruction, and show how it can be applied to real system.

2. We combine the method with machine learning, and present results.

3. We explain our ideas how to validate features.

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Anomalous temperature behavior of dielectric permittivity of magnetic fluoroperovskites as a prove of their intrinsic structural instability

SCIENTIFIC ORGANIZATION

Ioffe Institute

ABSTRACT

Temperature dependences of the dielectric permittivity of a group of intrinsically unstable antiferromagnetic and diamagnetic fluoroperovskites were investigated. All of the studied compounds reveal distinctly different behavior. We attribute the steady increase of the dielectric permittivity to the growth of the lattice instability of cubic fluoroperovskites at low temperature.

KEYWORDS

Ferroics, fluoroperovskites, dielectic permittivity, lattice instability.

ACKNOWLEDGEMENTS

This work was supported by the Russian Government Program P220 (Grant No. 14.B25.31.0025), by the Russian Foundation for Basic Research (Grant No. 15-02-04222), and by the Russian Scientific Foundation (Grant No. 16-12-10456).

SUMMARY

The search for new multiferroics and magnetoelectrics with efficient susceptibilities is one of the hottest topics in the today's condensed matter physics and material science. This task requires deeper understanding of the microscopical mechanisms of interaction between the lattice, orbital, and spin systems, and therefore combined efforts of both experimentalists and theoreticians are due. Here we report and analyze results of the dielectric permittivity studies of a group of intrinsically unstable antiferromagnetic and diamagnetic fluoroperovskites. The group includes four cobalt fluoroperovskites $KCoF_3$, $RbCoF_3$, $NaCoF_3$, and K_2CoF_4; the first two compounds experience antiferromagnetic and structural phase transitions, the last two only antiferromagnetic transition. For comparison, we also studied $KNiF_3$ which is antiferromagnetic below T_N = 246 K; no phase transitions take place in $KMgF_3$ and $KZnF_3$. The dielectric permittivity was studied as a function of temperature in the range of 4 – 350 K and in frequency range of 1 kHz – 1 MHz. Remarkably, all the studies compounds reveal distinctly different behavior. In $KCoF_3$, a noticeable increase of the dielectric permittivity of about 3.3% was observed when lowering the temperature. Moreover, only in $KCoF_3$, this behavior was superimposed by a broad peak near T_N = 115 K which we attribute to the previously observed strong magnon-phonon interaction in the vicinity of Brillouin zone center. Surprisingly, a very different temperature behavior of the dielectric permittivity was observed in $RbCoF_3$ with magnetic and crystallographic properties very similar to those of $KCoF_3$. In antiferromagnetic $KNiF_3$, and diamagnetic $KMgF_3$ and $KZnF_3$, a similar behavior was observed at low temperature with an increase of the dielectric permittivity of about 1-3%. We attribute the steady increase of the dielectric permittivity to the growth of the lattice instability of cubic fluoroperovskites at low temperature. Distinctly different behavior was observed in the orthorhombic $NaCoF_3$ and uniaxial K_2CoF_4 and this allowed us to conclude that the lattice instability is suppressed when the cubic structure of fluoroperovskites is broken. Consequently, no increase of the dielectric permittivity at low temperature found. We discuss recent ab initio calculations of potential multiferroics among fluoroperovskites. We consider that our findings may serve for better understanding of involved microscopic mechanism of multiferroicity and should help in efforts of searching pathways for creating new multiferroics among fluoroperovskites and other materials.

ADDITIONAL INFORMATION

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Analytics-Based Numerical Method for Signal Evolution in Fiber Lasers

SCIENTIFIC ORGANIZATION

Novosibirsk State University

ABSTRACT

Design of modern fiber lasers require massive numerical modelling because of multiple system parameters and complex nonlinear nature of light dynamics in the cavity. Therefore, analytical results for the light evolution in laser cavities are useful for optimisation and understanding of the underlying dynamics. The analytical solution for power evolution in general effective two-level active medium can be used in a combination with the amplitude field modelling allowing to reduce by orders of magnitude the simulation time by eliminating the first iterative procedure.

KEYWORDS

Fiber laser, signal evolution, doped fiber, signal gain.

ACKNOWLEDGEMENTS

The authors acknowledge financial support from the Ministry of Education and Science of the Russian Federation (14.B25.31.0003).

SUMMARY

Design of modern fiber lasers require massive numerical modelling because of multiple system parameters and complex nonlinear nature of light dynamics in the cavity. Therefore, analytical results for the light evolution in laser cavities are useful for optimisation and understanding of the underlying dynamics [1].

The analytical solution [2,3,4] for power evolution in general effective two-level active medium can be used in a combination with the amplitude field modelling allowing to reduce by orders of magnitude the simulation time by eliminating the first iterative procedure. We consider signal evolution in an effective two-level gain model [1].

For description of the signal gain in the doped fiber the analytical solution of an effective two-level system model is used. Based on this solution, the numerical method for signal evolution was designed for different resonator types. This method includes the separation of two iterative processes of the average power and signal settling, which accelerates the computational process and gives an optimization flexibility.

The analytical solution [2,3,4] allows to describe and study the generation start. Also this result can be generalized for assessing the output signal power for different resonator types, that can be useful at initial steps of the amplifying devices design.

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K-conductivity in solids: combined topological and density functional theory analysis

SCIENTIFIC ORGANIZATION

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ABSTRACT

The possible solid electrolytes chosen from the topological point of view were modelled at the first principles description level in order to investigate the values of activation energy barriers for potassium ions migration pathways. For this purpose the nudged elastic band method as it is implemented in CP2K package was used and resulted in low computer time consumption. After that the obtained activation energy barriers were used to conclude about the energetic/dimensional properties of ions diffusion nets in the substances are under consideration.

KEYWORDS

Potassium conductivity, solid electrolytes, ToposPro, topological analysis, CP2K, density functional theory, nudged elastic band.

SUMMARY

The solid state electrolytes based on K^+ conductivity are considered as main parts of the possible electrochemical devices. The topological analysis of the known K-containing structures can be used to select substances with respect to presence of migration pathways in a structure. One of the possible ways to predict K^+-conducting substances with the appropriate conducting properties is an application of the combined geometrical/topological approach. The latest allows to obtain net of voids in the structure causes cations diffusion, its size and dimensionality properties and connectivity. Recently, the Voronoi–Dirichlet partition-based approach was applied for prediction of the possible sodium conducting materials [1]. *ToposPro* [2] program package is able to perform such analysis for thousands of the known structures (e.g. collected in ICSD) are corresponding to the compositions and stoichiometry requirements. However, a final set of compounds available after that step is often enormously vast to have some experimental checking possibility.

On the other hand, quantum mechanical *ab initio* calculations are applied widely for the studying of the crystal structure and properties in the equilibrium states as well as in transitional ones. Permanent computer performance increase and a vast range of the possible implementations of the *ab initio* codes themselves have resulted in possibilities to investigate of the structures conduction properties by microscopic modelling. For this reason, it is possible to apply density functional theory-based calculations at the next stage of the selection in order to obtain ionic conducting properties (activation energies barriers) [3].

In the scope of the current research a number of potential solid electrolytes predicted by the mentioned above approach using *ToposPro* code were studied by the *ab initio* modelling in order to elucidate their ionic conducting properties which are not studied yet. Previously considered potassium and lithium conducting materials were studied additionally to validate the proposed approach by a comparison of the method predictions with the previous results.We use climbing image nudged elastic band method (CI-NEB) as implemented into the free-license *CP2K* code [4] and pay special attention not only to diffusion activation energies but also to relations between the vacancy formation energies to take into account not only geometrical but also energy favorability of some pathways.

Thanks to use of *QUICKSTEP* electronic structure calculation method [5] implemented in *CP2K* code based on the combined Gaussian and plane waves basis set it has become possible to study more than 65 different pathways for more than 10 structures. Additionally, the developed script-based system allowed to get result within the reasonable period of time using the SCTMS ‘Zeolite’ and ‘Sergey Korolev’ supercomputers at Samara University. It should be noted, that the applied method results a lower computer time consumption (in comparison with well-known pure plane-waves package, e.g. *VASP* [6]). This observation points possibilities to evaluate more complex doped as well as disordered electrolyte systems at the first principles level of description. That is extremely important for predictions of the particular doped electrolytes properties.

In result of the work, more than 30 activation energy values were calculated for five possible solid electrolytes chosen from the topological point of view with not known conducting properties. The obtained values were used to conclude about the energetic/dimensionality properties of K^+ diffusion in the substances are under consideration.

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Advanced post-processing procedure for industrial quantum key distribution systems

SCIENTIFIC ORGANIZATION

Russian Quantum Center

ABSTRACT

We report about the joint research project, which is aimed on a design of an industrial fiber based QKD system in Russia. The QKD engine is based on the decoy states BB84 protocol. We present the developed post-processing procedure for sifted quantum keys (i.e., keys after reconciliations), which consists of error correction, parameter estimation, and privacy amplification. Communications over public channel are authenticated.

KEYWORDS

Quantum cryptography, quantum communications.

ACKNOWLEDGEMENTS

The support from Ministry of Education and Science of the Russian Federation in the framework of the Federal Program (Agreement 14.579.21.0104) is acknowledged.

SUMMARY

Great attention to quantum key distribution (QKD) systems is related to the fact of breaking of public-key encryption algorithms using quantum computing. Security of public-key exchange schemes can be justified on the basis of the complexity of several mathematical problems. Nevertheless, the Shor’s algorithm allows solving these problems in a polynomial time. Absence of efficient classical (non-quantum) algorithms breaking public-key cryptosystems still remains unproved.

In this contribution, we report about the joint research project, which is aimed on a design of an industrial fiber based QKD system in Russia. The QKD engine is based on the decoy states BB84 protocol. We present the developed post-processing procedure for sifted quantum keys (i.e., keys after reconciliations), which consists of error correction, parameter estimation, and privacy amplification. Communications over public channel are authenticated.

The post-processing procedure works as follows [1]. Sifted keys go through the error correction that is adjusted on the current value of QBER. After accumulation of necessary number of blocks they input to the parameter estimation (together with their versions before the error correction).

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ADDITIONAL INFORMATION

Dear organisers, Our contribution is a part of the innovative project on a design of industrial quantum key distribution systems. The first system of a such a kind in Russia. These systems uses number of technologies, which are on the frontiers of optoelectronics, photonics, engineering, and quantum technologies. This is a large project with both scientific and engineering backgrounds, and, it has a commercial output. Our results have been largely covered by mass media (http://www.forbes.ru/tekhnologii/tekhnika-i-biznes/319925-zachem-banku-fiziki-gazprombank-stal-krupneishim-investorom-ros; http://www.vedomosti.ru/technology/articles/2016/06/16/645511-gazprombank-kvantovii-tsentr; http://ria.ru/science/20160609/1444994358.html; http://ria.ru/science/20160616/1447918030.html; http://bosfera.ru/bo/kvanty-reshayut-vsyo). Hereby, I would like kindly ask you to consider possibilities to present our results not in the framework the poster session, but as a talk. In this way, I'm sure presentation of our project will be a substantial part of this great event. With kind regards, Authors

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RIN transfer induced signal degradation in fiber optical communication links

SCIENTIFIC ORGANIZATION

Novosibirsk State University

ABSTRACT

This work is devoted to mathematical modeling of signal degradation in fiber optical communication links. We use the method of mathematical modeling based on non linear Shrodinger equation (NLSE) to investigate relative intensity noise(RIN) transfer in Raman fiber amplification systems. We demonstrate the calculation method of the RIN Transfer function within the NLSE based models and application of this methods to the study of the signal degradation problems.

KEYWORDS

Fiber optical communication links, distrubuted Raman amplification, relative intensity noise (RIN), RIN Trasnfer, four-wave mixing.

ACKNOWLEDGEMENTS

The work is supported by Russian Science Foundation (grant 14-21-00110).

SUMMARY

It is well known that degradation of an information signal during its propagation along the fiber optical communication link can significantly restrict bit rate. In practice, any real transmission link introduces distortions into the signal that can be either recoverable (e.g., dispersive broadening) or not fully removable (e.g., noise). The sources of such unremovable distortions leading to loss of information are double Rayleigh scattering (DRS), amplified spontaneous emission (ASE), RIN (Relative Intensity noise transfer) and nonlinear interactions such as four-wave mixing

FWM [1]. Recently many works investigated RIN Transfer from pump to signal in Raman fiber lasers and amplifiers both numerically [2,3]

and analytically [4]. However, analytical models work only in the case of undepleted pump approximation, which is not always satisfied in the real communication links. Moreover, the most common analytical and numerical models are based on balance (average-power) equations and do not describe evolution of phase modulated signals along the fiber under influence of dispersive and nonlinear effects. To investigate RIN transfer in the real Raman fiber amplification systems we perform a numerical modelling based on a generalized nonlinear Schrödinger equation taking into account dispersion, Kerr nonlinearity and Raman gain. We develop a method of RIN transfer calculation in the amplitude models and use this method to study signal degradation. We numerically investigate phase-modulated signal degradation due to RIN transfer in the real optical communication link and show that not only Raman scattering but also FWM can initiate pump to signal intensity noise transfer.

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Physics and unified technology platform of intense ultrafast optics for avionics, medicine and nanophotonics

SCIENTIFIC ORGANIZATION

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ABSTRACT

The next key enabling technologies are developing in the project: Technology of optical fibers and fiber components for ultrafast applications. Technology of power scaling of ultrafast lasers using high-power optical amplifiers. Technology of THz emitters using semiconductor disk lasers and effect of modulation instability. All these technologies are used to develop all-fiber sub-picosecond laser systems with ultra-high peak power. The applications of the developed pulsed systems in medicine, avionics, communications, material processing are investigated.

KEYWORDS

fiber lasers, semiconductor disk laser, ultrashort intense laser pulses, THz emitters, tapered fibers, high threshold of stimulated Brillouin scattering, LIDAR, lasers for bio-medical applications.

ACKNOWLEDGEMENTS

Ministry of Education and Science of Russia.

SUMMARY

The invention of the laser triggered a non-stop development of principally new types of devices, engineering systems and innovative techniques with an enormous range of scientific and technological applications and corresponding impact on society from the Internet to medical laser applications. Nowadays, lasers have become ubiquitous devices equally important in fundamental science, engineering technologies and in a range of practical applications. In the last decade there has been a revolutionary progress in laser science fuelled by advances in high-power systems, ultra-short pulse lasers and oscillators with high pulse energy. The progress was driven by a variety of new important applications that these advanced laser systems can open-up. This expansion has been facilitated by continuous advances in material science, achievements in technology and by the improvement in our understanding of the fundamental laser principles and physical effects underlying the operation and performance of new types of lasers. In particular, laser

designs based on new physical concepts offer opportunities for creating systems with non-incremental changes of performance characteristics leading to disruptive progress in middle and long term prospects.

Our current project aims for a breakthrough in laser science and technology through development of a radically new concept of laser employing special optical fibers with key parameters varying along the fiber length. On this way fiber laser systems with record performance characteristics have been designed and employed for several applications in material processing, ranging sensing and medicine.

Success of the project is predetermined by particular scientific and technical contributions made by our team to the following areas:

- advanced understanding of light interaction in optical fibers with special properties
- novel light sources with tailorable temporal, spectral, and statistical characteristics
- new fiber materials and structures with enhanced functionality
- urgent photonic applications

Here we highlight the main scientific achievements:

- Employing a number of special fibres all-fiber sub-picosecond systems have been demonstrated for operation at 1.06 μm and 1.55 μm achieving a peak power up to 1MW.
- New universal model describing chirped pulse propagation in longitudinally non-uniform fibers taking into account effects of modulation instability, cross-phase modulation and Raman scattering has been developed and resulted in the designer software allowing an accurate analysis of pulse temporal dynamics (soliton collapse, bound-states of high energy solitons) as well as nonlinear spectral compression in fibers of different geometry.
- New concept of soliton management in fibers with variable dispersion has been proposed and applied for design of new photonic devices:
    - optical pulse compressors
    - pulse train generators with repetition rates higher 100 GHz
    - broadband supercontinuum sources covering an octave in spectrum domain

New master oscillator - power amplifier system based on erbium-doped fibers comprising all these elements has been built and tested demonstrating an advance of the developed concept.

- Ultrafast pulse train generators based on passively mode-locked semiconductor disk lasers has been demonstrated and tested for operation with output power above 100 mW.
- A technology for fabrication of longitudinally non-uniform active and passive optical fibers with high Brillouin threshold has been elaborated. The designer software has been developed to control the fabrication process.
- High power narrow bandwidth laser generator based on a tapered fiber has been designed and applied for the LIDAR system providing the advanced performance characteristics:
    - optical linewidth – < 6 kHz,
    - pulse energy – above 3 μJ,
    - pulse duration – 10-100 ns
- A family of fiber lasers for bio-medical applications has been offered and applied to study in vivo the effect of laser radiation on biological specimens:
    - 1264-1270 nm sub-picosecond laser with peak power up to 25 kW
    - Er-Ho doped fiber laser with pulse duration of 1-10 ps and peak power up to 10 kW
    - picosecond fiber laser tunable over spectrum range from 1550 to 2100 nm
    - picosecond Ho-doped fiber laser system with peak power over 10 kW

- The picosecond laser system based on ytterbium-doped fiber has been tested for operation with peak power higher than 1 MW and applied for nanostructuring of metal and semiconductor surfaces. In particular, inscription of periodic structures with sub-wavelength spatial resolution has been demonstrated.

In next few years, the proposed concept and the results of the project have to trigger technological breakthroughs in many areas of science and engineering and will lead to particularly strong impact on optical fiber communications, fiber sensing and microwave photonics.

Among the tasks addressed to the next years of the project are:

- Extension of the developed concept to new fiber materials, including Bi-doped, Tm-doped optical fibers, chalcogenide fibers, photonic crystal fibers, and endlessly single mode fibers providing advanced diversity of the generation wavelength (in the range covering 1 - 2.5 μm) and controllable nonlinearity of light-matter interaction
- Extension of the developed concept to plasmon-polariton dynamics providing generation, amplification and control of the plasmon-polariton waves through light-matter interaction in layered structures. The idea of plasmon wave amplification by the drift currents and electronic beams will be also developed.
- Design and application of new laser sources for range sensing and free-space communication. In particular, lasers operating at ~2.1 μm will be developed and applied for this concern.
- Design and application of new laser sources for in vivo bio-medical experiments. In particular, the effects of laser radiation at new wavelengths on an oxidant stress in cancer cells will be evaluated for most efficient cancer treatment.
- Harnessing of stimulated Brillouin scattering in special fibers for recording of dynamical Brillouin gratings with advanced performance characteristics. Studies and design of narrow-band Brillouin laser sources (<1kHz) based on dynamical Brillouin gratings.
- Application of the developed narrow-band Brillouin lasers for distributed fiber sensing, elaborating advanced functionality and low-cost solutions for optical sensors used in oil and nuclear industries, building construction, municipal services.
- Development of nonlinear optical circuits realizing conversion of CW laser radiation into ultra-fast pulse trains (~1 THz and higher). The effects of modulation instability and four-wave-mixing taking place in circuits comprising fiber lasers, disc lasers and surface plasmonic devices (nano-antennas) will be implemented for this purpose. Applications of such generators for telecommunication, metrology and security systems will be considered.
- Design and application of new photonic devices for microwave photonics - systems of generation, transmission and analysis of the microwave signals. In particular, ultra-narrow-band RF generators operating at GHz - THz will be designed and tested. Studies of dynamical Brillouin gratings will result in design of cost-effective Instantaneous Frequency Measurement (IFM) system (widely tunable narrow-band RF filters) that is of critical importance for RF signal processing.

In general, the scientific problems considered in the project are related to technologies that are promising for future optoelectronic designers all over the world. The integration of the developed circuits will allow the development of competitive devices demanded by security sector, oil industry, nuclear power industry, telecommunications, biochemistry and medicine.

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Collisions of coherent structures and formation of rogue waves in NLSE

SCIENTIFIC ORGANIZATION

Novosibirsk State University

ABSTRACT

In this work we present numerical simulation of modulation instability of the condensate and cnoildal wave. For this experiments we discuss probability of rogue waves formation from randomly perturbed initial conditions in terms of breathers collisions. We propose different statistical models of solitonic and breathers gas. One of this models is based on our recent work devoted to the theoretical and experimental study of the so called super-regular NLSE breathers which play a special role in the NLSE dynamics.

KEYWORDS

Solitons, nonlinear waves.

ACKNOWLEDGEMENTS

The authors thank for the support of the Russian Science Foundation (Grand No. 14-22-00174).

SUMMARY

Collisions of coherent structures such as solitons or breathers is the main mechanism of rogue waves formation in the nonlinear Schrodinger equation (NLSE) and other integrable systems. The statistical description of this process is the question of great importance for the practical applications and for the theory of integrable turbulence [1]. The full integrability of NLSE gives enormous advantages for the construction of the theory for rogue waves formation. Using the inverse scattering transform one can analyse wave field in terms of spectrum for the Zakharov-Shabat system. It allows to distinguish coherent structures and to predict properties of their collitions.

In this work we present numerical simulation of modulation instability of the condensate and cnoildal wave [1,2]. For this experiments we discuss probability of rogue waves formation from randomly perturbed initial conditions in terms of breathers collisions. We propose different statistical models of solitonic and breathers gas. One of this models is based on our recent work devoted to the theoretical and experimental study of the so called super-regular NLSE breathers [3,4] which play a special role in the NLSE dynamics.

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ADDITIONAL INFORMATION

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Wide Band Gap Semiconductors

SCIENTIFIC ORGANIZATION

Centre National de la Recherche Scientifique

ABSTRACT

Realization of LEDs operating indeep UV is tricky as the issue is the control of the p-type doping of aluminium-rich AlGaN. Boron nitride is naturally p-type an alternate for realizing hole injection. Realizing optoelectronic devices that combine wurtzitic nitrides with a hexagonal crystal is however a multiple hurdle race. The recent growth of h-BN films by metal-organic vapour epitaxy without PL at 5.5 eV is an indicator of a really very good quality. This indicates that the quality of h-BN epi-layers is now mastered and that this material is in its way for application in the UV.

Keywords

Optical properties of BN for UV emission.

Acknowledgements

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Summary

While discovering in 1986 that the growth of a low temperature buffer layer at the interface with the sapphire substrate was improving the performances of GaN, Nobel Prizes Isamu Akasaki and Hiroshi Amano, as well as their collaborators of Nagoya probably did not realize how impacting would be this discovery.

A couple of years later, after that they had managed to control both p-type and n-type dopings, they realized the first GaN-AlGaN light emitting diode (LED) . Hundreds of different devices derive from their pioneering works at the Meijo and Nagoya universities.

The opto-electronic market now overlaps with the huge market of solid state lighting, based on the utilization of blue light emitters coupled to yellow light emitting phosphors.

Although the yield of such LEDs is very good in the blue, the supremacy of the nitride technology is more difficult to establish at both sides, namely in the green and ultra violet (UV) wavelength regions. The reasons for these difficulties have different origins. In case of devices that would fill the green gap, it is mandatory to grow very high quality indium-rich alloys so that non radiative recombination rates are almost eradicated and no longer compete against the radiative recombination rate. Regarding the deep UV, the dominating issue is the control of the p-type doping of aluminium-rich AlGaN alloys and their valence band physics.

Boron nitride is an alternate for realizing hole injection. Realizing optoelectronic devices that combine wurtzitic nitrides with a hexagonal crystal is however a multiple hurdle race. Researchers are facing many challenges but the recent growth of h-BN films by metal-organic vapour epitaxy (MOVPE) (Appl. Phys. Lett. **108**, 052106, 2016) indicates that scientists are probably on the good way.

In this communication we demonstrate the indirect nature of the band gap of h-BN using one-photon and two-photon cw photoluminescence, photoluminescence excitation spectroscopy and time-resolved photoluminescence in the 8K-300K range, using bulk h-BN crystals commercialized by hqgraphene (www.hqgraphene.com). We demonstrate the specificity of the indirect band gap (valence band maximum at K point of the first Brillouin zone, and conduction band minimum at M) and we identify different phonon-assisted transitions and their overtones. The indirect exciton binding energy is found to be about 130 meV (Nature Photonics 10.1038/nphoton.2015.277). We demonstrate that the strong, lower energy (about 5.5 eV) lu-

minescence lines result of a cascade of TO(K) phonon-assisted intervalley scattering processes stimulated by defects of the crystal (Phys. Rev. B **93**, 035207,2016).

This permits us to claim quantitatively, based on our study that the absence of such PL at 5.5 eV in the MOVPE crystals referred above is an indicator of a really very good quality. This indicates, we believe it: *i*) that the quality of h-BN epilayers is now mastered and *ii*) that it is interesting and *iii*) that this material is in its way for application in the UV. Time has now come for it to be more deeply investigated, in particular by device growers.

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Analytical theory of blowout regime in radially inhomogeneous plasmas

SCIENTIFIC ORGANIZATION

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ABSTRACT

An analytical model for beam loading in a bubble generated by a short laser pulse or a relativistic electron bunch in radially inhomogeneous plasmas is developed. The influence of an arbitrary electron bunch on the bubble shape is described. The bunch profile needed to produce a homogeneous accelerating field is also calculated. Our results are applied to deep plasma channels with various radial density profiles, namely, power-law and step-like. The model predictions are verified by 3D particle-in-cell simulations and are in good correspondence with them.

KEYWORDS

Plasma wakefield, bubble regime, electron acceleration, plasma channels

ACKNOWLEDGEMENTS

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SUMMARY

Introduction

Lately a lot of attention has been given to plasma acceleration methods [1, 2] in which an intense laser pulse or a bunch of charged particles is used to excite a plasma wakefield whose large longitudinal field is used for acceleration. Such methods provide acceleration rates orders of magnitude higher than conventional methods. So far electron bunches with the energy up to 4.2 GeV at the acceleration distance of 9 cm have been observed in experiments [3] for laser-wakefield acceleration (LWFA), while for plasma-wakefield acceleration (PWFA) the possibility of energy doubling from 42 GeV to 85 GeV at a distance of approximately one meter has been demonstrated [4].

One of the most promising regimes of plasma acceleration is the so-called “bubble” or “blow-out” regime in which electrons behind the driver are almost completely expelled and a spherical plasma cavity free of electrons is formed [5]. This cavity is usually called “bubble” On its border a thin electron sheath consisting of the expelled electrons is created. The cavity itself travels with near-luminous velocity through the plasma. The longitudinal electric field in it is uniform is the transversal direction, while the focusing force acting on the accelerated electrons is linear in radius and uniform along the cavity. In spite of the fact that this regime provides large acceleration gradients, obtaining electron bunches with low emittance, low energy spread, and high stability is a challenging task. One of methods of improving the bunch quality is using deep (or hollow) channels in plasma. The lack of ion column at the axis for such kind of channels significantly reduces the focusing force acting on the electrons, while, for the case of LWFA, the parameters of channel also provide additional freedom for balancing between the laser depletion and dephasing lengths. The possibility of obtaining electron bunches with the energy of 7.5 GeV and the energy spread of only 0.3% in a plasma with a deep channel has been shown in numerical simulations [6]. Due to the complexity

of the strongly nonlinear “bubble” regime of the plasma wakefield it is commonly studied using 3D particle-in-cell (PIC) simulations. But its theoretical description is also of considerable interest. However, all recent theories address only the case of homogeneous plasmas, which cannot be applied to the case of plasmas with channels.

Here we develop a generalized theory analytically describing the bubble envelope for plasmas with arbitrary cylindrically symmetric plasma profiles [7]. This theory is based on the theory for homogeneous plasma by Lu et al. [8].

Model of a strongly-nonlinear wakefield

To develop a general model we assume that a laser pulse or a relativistic electron bunch is propagating through the plasma along the axis z and is exciting a wakefield in the strongly-nonlinear regime in it. The plasma is described by its radially symmetric ion density profile $\rho_i(r)$. As the structure of the wakefield slowly changes during its propagation through the plasma, the quasi-stationary approximation, under which all values depend only on the difference $\xi = t - z$ between the time and longitudinal coordinate, is also assumed.

In our theory the following phenomenological model of a bubble is used: inside the plasma cavity there is no plasma electrons left, outside it the plasma is non-perturbed, while on its border, which is described by a function $r_b(\xi)$, there is a thin electron sheath of small constant width Δ. Using this model the following wakefield potential can be obtained inside the bubble:

$$\Psi(r,\xi) = \Psi_0(\xi) - \int_0^r S_i(r')r'dr',$$

where $S_i(r) = \int_0^r \rho_i(r')r'dr'$.

The wakefield potential is defined as $\Psi = \varphi - A_z$, where φ is the electric potential and A_z is the longitudinal component of the vector-potential (the Lorenz gauge is also assumed). Using this expression for the potential as well the expression for the radial component of the vector-potential A_r, it is possible to calculate the fields inside the bubble and therefore to describe the electron motion.

As the bubble sheath consists of electrons, its inner border is also an electron trajectory, which allows to find an equation for the bubble’s envelope:

$$A(r_b)r_b'' + B(r_b)r_b' + C(r_b) = \lambda(\xi)/r_b.$$

The source $\lambda(\xi)$ in the RHS of this equation depends only on the radial coordintate. When the width of the electron sheath is small and the bubble is large

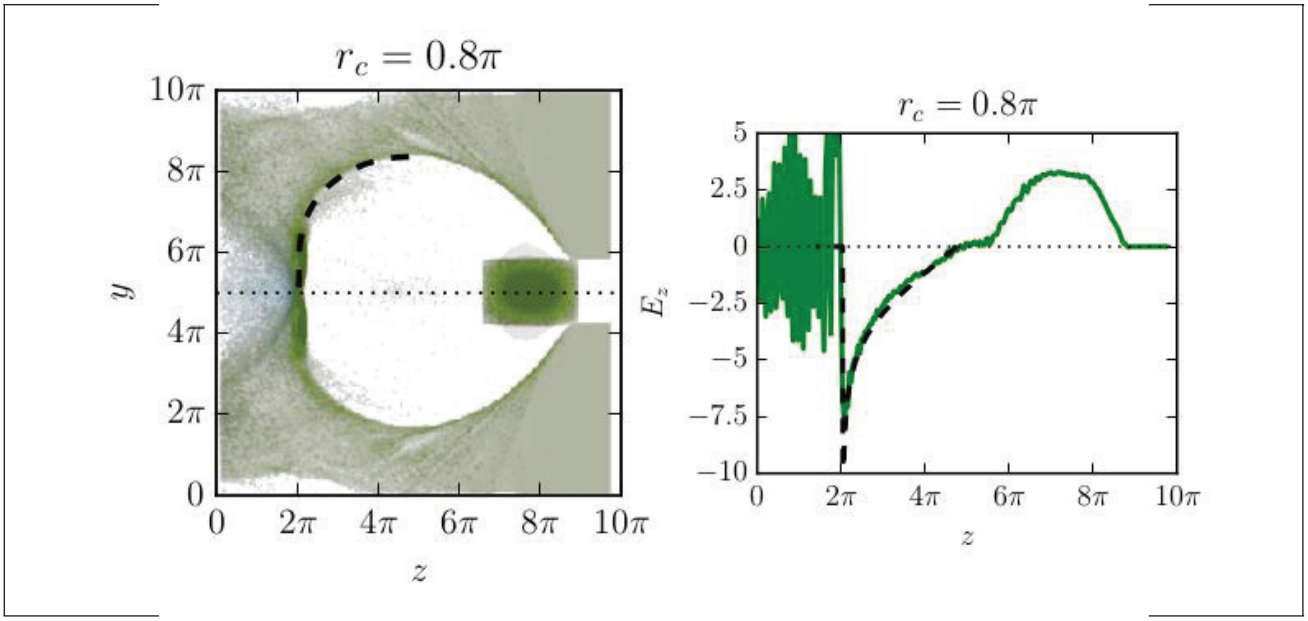

FIG. 1. Electron density distributions and corresponding longitudinal electric field profiles on the axis of the bubbles as observed in PIC simulations for different channel radii r_c. Analytical solutions for the bubbles’ shapes and the fields in them are shown with the dashed lines.

enough, the coefficients of this equation depend only on the plasma profile $\rho_i(r)$. The comparison of analytical solutions found by using this equation to the results of 3D PIC simulations (Fig. 1) shows that the model correctly describes both the shape of the bubble and the longitudinal electric field in it.

Homogeneous accelerating field by the adjustment of the accelerated bunch profile

The model also allows to describe plasma cavities with arbitrary electron bunches. In order to improve the quality of the accelerated bunch it is necessary to have homogeneous accelerated field in the whole volume of the bunch. Transverse homogeneity of this field is always present in the scope of this model, therefore it is required only to obtain longitudinal homogeneity. It can be shown that this field cannot be homogeneous in a non-loaded bubble (i.e. a bubble without an accelerated bunch). However, the accelerated bunch itself affects the shape of the bubble, therefore we may try obtaining homogeneous longitudinal field by ajusting the profile of the bunch $\lambda(\xi)$.

It turns out that it is possible to do for an arbitrary plasma profile. The resulting electron bunch profile is close to trapezoidal in the trasverse direction. In order to verify that such electron bunch can provide homogeneous longitudinal electric field, we have carried out 3D PIC simulations (Fig. 2). The results of these simulations have been compared to the predictions of our theory. It is indeed visible that the accelerated bunch deforms the shape of the bubble in such a way that the longitudinal field is uniform along the bubble.

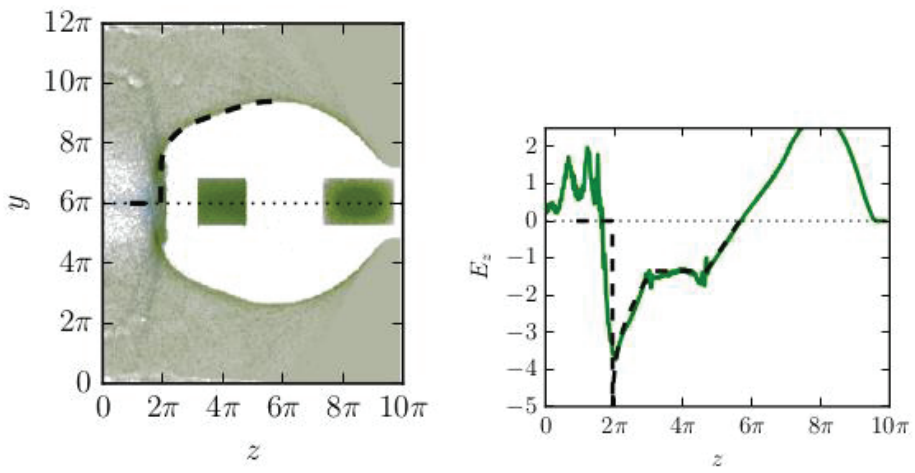

FIG. 2. Electron density distributions and corresponding longitudinal electric field profiles on the axis of the bubbles for an accelerated electron bunch with the necessary profile. Analytical solutions are shown with the dashed lines.

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The investigation of the switching of ferroelectric films BiFeO3 by second harmonic generation optical microscopy in a planar pattern of electrodes

SCIENTIFIC ORGANIZATION

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ABSTRACT

The polarization switching in ferroelectric films with a planar periodic electrodes structure has been investigated. The local polarization distribution in an interelectrode gap of these films in an applied electric field has been studied by nonlinear optical microscopy. The polarization switching parameters showed the high inhomogeneity of the polarization distribution in studied structure.

KEYWORDS

BFO nonlinear optics polarization switching SHG microscopy

Acknowledgements

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SUMMARY

In the most ferroelectric devices there used polarization switching in the direction which is perpendicular to the film plane. Planar geometry is optimal for the optical applications because it guarantees more effective interaction of electromagnetic wave and ferroelectric polarization as well as gives wide opportunities for elements integration and creation of the new generation of optical IC.

The switching of ferroelectric films BiFeO was investigated by second harmonic generation microscopy in a planar pattern of electrodes. Investigation data turned out indispensable for the revelation of the electric field distribution in the structure.

Figure 1. Nonlinear optical image (mapping) of the BFO film with planar pattern of electrodes for different values of applied field: -25V (a), 0V (b), +25V (c), 0V (d). Image (a) shows the highlighted areas for which there was conducted an analysis of the switching parameters in local area.

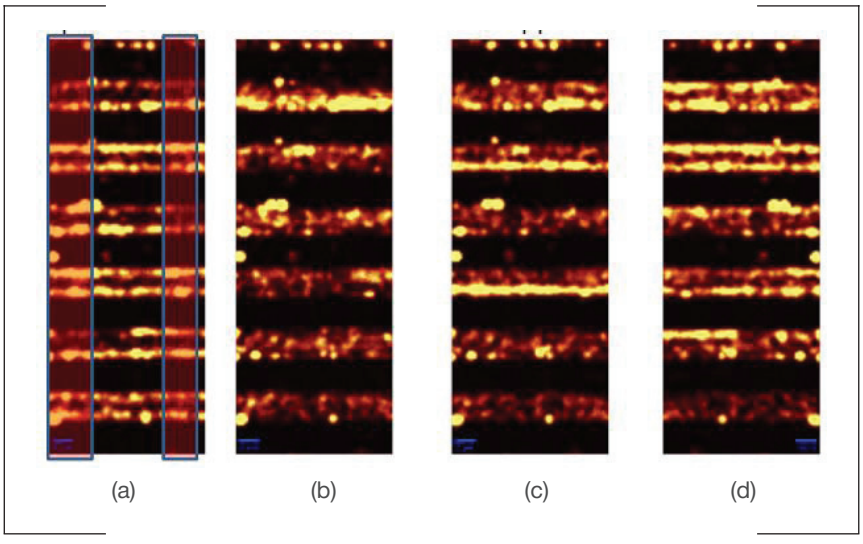

Figure 2. Cross-section of nonlinear optical images built in selected areas for different parameters of applied field.

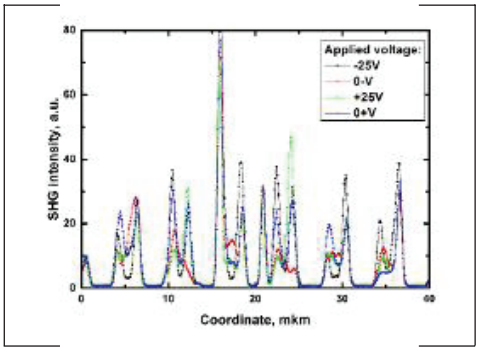

Figure 1 represents the results of nonlinear optical mapping of ferroelectric films BiFeO3 when applying electric field to a planar pattern of electrodes with the range of 2 mkm and the width gap of 2 mkm.

As we know from the [1] the intensity of the SHG signal which is generated by metallic electrodes is very small in comparison with SHG intensity from the ferroelectric films especially when applying electric field. That's why dark areas on the nonlinear optical image can be identified as electrodes.

It was shown in the [1], that the SHG intensity is proportional to ferroelectric polarization square, representing the sum of polarization terms depending and independing from the external electric field. SHG intensity will be equal when applying electric field with different signs with the small part on the unswitching polarization and it will be impossible to define oppositely polarized area on nonlinear optical image.

From the figure 1 it is obvious that the structure contains relatively big parts of unswitching polarization which may be linked to the formation of different kind defects (including mechanical strain) in near-electrode area.

Figure 2 represents cross-section built in selected areas. It is seen that local switching parameters shows the high inhomogeneity of the polarization distribution in studied structure.

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Phase transition in HTB-FeF3/rGO cathode material: x-ray spectral diagnostics and ab inition modelling

SCIENTIFIC ORGANIZATION

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ABSTRACT

A porous framework of HTB-FeF3/rGO composite was used as conversion cathode material in Li-ion battery. Electrode shows a good cycle stability due to the intimate contact of FeF3 nanoparticles with graphene oxide. Using in situ XRD, XAS and Mossbauer spectroscopy, we show that during discharge of HTB-FeF3/rGO composite Li is intercalated into the tunnels of the HTB-FeF3 structure up to x=0.92 Li. Intercalation is followed by slow conversion of HTB-LixFeF3 to LiF and Fe nanoparticles. During charge, the LiF and Fe phases are slowly transformed to amorphous FeF2 and FeF3 phases.

KEYWORDS

Conversion materials, DFT, evolution algorythm, XANES, EXAFS, XRD, fluorides.

ACKNOWLEDGEMENTS

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SUMMARY

In our study we pursue the goal to determine structural changes which take place inside the full Li-ion cell and to look at those processes in situ during cycle. Experiment was carried on the B station of BM01 (SNBL) beamline at ESRF, Grenoble, as a mixed XAFS/XRD experiment. Samples were prepared with synthesis of iron fluoride nanoparticles inside reduced graphene oxide sheets which increases conductivity. The material offers a stable discharge energy of 600-700 Wh/kg over 100 cycles, which is higher than the widely applied cathode materials (300-500 Wh/kg). Each sample we cycled with 20 mAh/g in the 1,2-4,2 V range, while measuring Fe K-edge XAFS spectra in transmission mode and XRD patterns with 15 minutes interval. For measurements we used self-made test cells with glassy carbon windows connected to Gamry potentiostats responsible for cycling and data acquisition.

Results of the x-ray studies were associated with cycling data to obtain structure-charge state dependency. HTB structure of the as-prepared material has open intercalation channels as a result, full electrochemical reaction can be separated into initial intercalation of one Li- anion per formula unit and following conversion reaction involving two more Li-, which gives us 3LiF/Fe mixture and a complete three electron transition. To prove this we performed principal component analysis (PCA) on the series of XAFS experimental spectra. We have used FitIt software to mathematically decompose the series of the Fe K-edge spectra at different voltages into independent sub-spectra. It was found that all spectra for discharge process can be reproduced as a combination of three components. First component corresponds to HTB structure, second to the intercalated structure with Fe2+

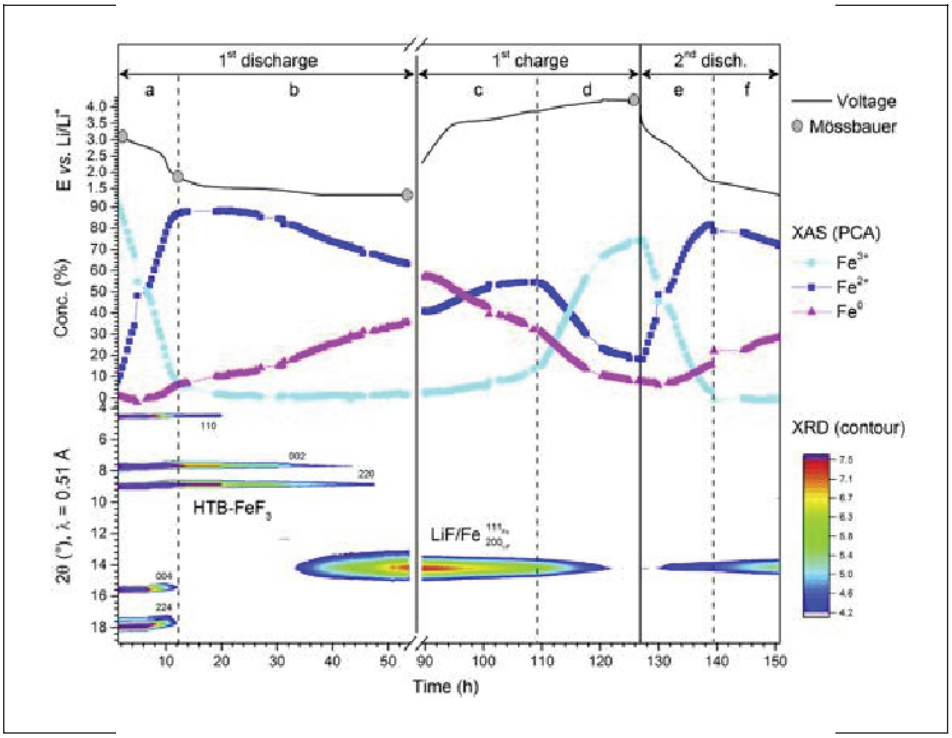

Figure 1. In situ XAS/XRD experiment of HTB-FeF3/rGO composite. Top: Voltage profile during charge/discharge of the cell with grey circles indicating points where ex situ Mossbauer spectra were collected. Middle: PCA concentration profile of Fe, Fe2+ and Fe3+ components obtained from simultaneous decomposition of 260 Fe K-edge XANES spectra. Bottom: XRD contour plot (lambda=0.51 Å) showing evolution of HTB-FeF3, LiF and Fe phases during charge/discharge.

charge state and the third one corresponds to metallic Fe. We have observed that pure iron nanoparticles form after HTB conversion to intercalated phase. We have performed a set of ab initio calculations using evolutionary algorythms (USPEX software) within pseudopotential DFT approximation (VASP 5.2) to analyse phase transition in FeF3 material upon intecalation and conversion regimes.

The good cycle performance of the material was attributed to the microstructure, which consists of FeF3particles embedded into a matrix of graphene oxide. The close contact of hygroscopic FeF3particles with carbon permits the preparation of high quality electrodes without the need

of moisture protection in ambient air and maintains electronic as well as Li ionic conductivity during prolonged cycling. The detailed reaction mechanism was investigated using a combination of in situ methods. Upon discharge, Li is inserted fast into the HTB-FeF3 tunnel structure followed by a slow conversion reaction to LiF/Fe nanoparticles. Upon charge, LiF/Fe is slowly converted back to rutile FeF2 and amorphous FeF3 phases without reformation of the HTB-FeF3 framework.

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Sub-Thz Wave Generation by Plasma under High-Current Relativistic Electron Beam Impact in the GOL-PET Experiment

SCIENTIFIC ORGANIZATION

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ABSTRACT

Plasma emission in terahertz band during interaction of an intense relativistic electron beam with plasma is considerably interesting as bases for creation of high power generators. Strong plasma turbulence pumped by the beam at presence of magnetic field can generate EM-waves with frequencies close to upper-hybrid frequency and at its double value. To study this phenomena the specialized GOL-PET facility has been created with plasma Ne~10^15 cm-3 and the electron beam I~30 kA, E~0.6 MeV. Results of experimental studies of EM-wave generation will be presented in this paper.

ACKNOWLEDGEMENTS

RSCF under Project No. #14-12-00610.

SUMMARY

In the paper, last experiment's results on sub-THz wave emission from the area of relativistic electron beam-plasma interaction in the GOL-PET device are described [1]. A plasma column with the diameter of 6 cm, length of 2.5 m and its density (0.2-2) x10^{15} cm^{-3} is confined by multiple-mirror magnetic field with mean value of 4 T. The electron beam (REB) injected into the column, has the following parameters: energy E_b ~ 0.8 MeV, current I_b ~ 30 kA, current density J_b ~ 2 kA/cm^2 in the mean magnetic field. Previous studies [2] have shown that the beam is pumping the plasma electron oscillations in a vicinity of the upper hybrid wave branch. These plasma oscillations can be converted in electromagnetic waves on regular or artificial plasma density gradients (the plasma radiation with the upper hybrid frequency). The electromagnetic waves with the double upper hybrid frequency are also generated in the beam-plasma system due to coalescence of the plasma oscillations in case of high level of the oscillation energy density.

The described experiments are devoted to measure the spectral properties of the generated radiation and the directions of the sub-THz plasma emission in depending on plasma and beam parameters. As results of these experiments, the wave emission with the specific power concentrated in the direction along the axis of the plasma column, in the frequency interval 0.25-0.5 THz has been obtained at the plasma density about of 10^{15} cm^{-3}.

This research was financially supported by RSCF under Project No. #14-12-00610 for the investigation of sub-terahertz emission from plasmas. The upgrade of the radiometric system was funded by the Ministry of Education and Science of RF under the State Assignment Contract No. #3002.

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Additional information

A.V. Arzhannikov, A.V. Burdakov, V.S. Burmasov, L.N. Vyacheslavov, I.A. Ivanov, A.A. Kasatov, S.A. Kuznetsov, M.A. Makarov, K.I. Mekler, S.V. Polosatkin, V.V. Postupaev, S.L. Sinitsky, V.F. Sklyarov.

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Probability Distribution Functions of freak-waves

ABSTRACT

D.I. Kachulin, A.I. Dyachenko, V.E. Zakharov Presented are the results of numerical experiments on calculation of Probability Distribution Functions for surface elevations of water waves arising during the evolution of wave field which is described by JONSWAP spectrum.

KEYWORDS

Nonlinear water waves, Hamiltonian formalism, modulational instability, freak waves.

ACKNOWLEDGEMENTS

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SUMMARY

Considering surface gravity waves which propagate in same direction we apply canonical transformation to a water wave equation and drastically simplify the Hamiltonian. This transformation explicitly uses the vanishing exact four-wave interaction for water gravity waves for a 2D potential fluid. The simplification of Hamiltonian allows to derive new compact equation which solves the spatial Cauchy problem for surface gravity wave on the deep water. This new equation can be easily implemented for numerical simulation.

No doubts that estimation of probability of extreme waves, or freak-wave, appearing at the surface of ocean has practical meaning. They are a native part of the surface wave dynamics in the open seas, and amongst different mechanisms of this phenomenon, linear dispersion and modulational instability are generally recognized. In the frame of the new spatial equation we calculate PDF for surface elevations of water waves which is described by JONSWAP spectrum for different values of wind speed.

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Ultrafast optical control of magnetic anisotropy in metallic and dielectric thin films

SCIENTIFIC ORGANIZATION

Ioffe Institute

ABSTRACT

Femtosecond optical pulses provide unique opportunity to control the magnetic state of matter on pico- and subpicosecond timescale. Here we present the results of experimental studies demonstrating ultrafast control of magnetic anisotropy in metallic (Galfenol) and dielectric (iron garnets) thin magnetic films. We demonstrate that picosecond change of magnetic anisotropy is mediated by laser-induced heating or strain and triggers the magnetization precession in the studied films, which amplitude, frequency and initial phase can be tuned by external magnetic field.

KEYWORDS

Laser-induced dynamics, magnetic thin films, femtosecond magnetism, picosecond magnetoacoustics.

ACKNOWLEDGEMENTS

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SUMMARY

In recent years controlling magnetic state of matter by external stimuli, which duration is much shorter than the typical magnetic field pulses, became one of the primary goals in fundamental and applied magnetism. The most promising approaches allowing effective and fast control of magnetization utilize spin-polarized currents [1], picoseconds acoustic pulses [2] and, as the ultimate tool, femtosecond optical pulses [3,4]. All these stimuli, in particular, can trigger magnetization precession in magnetic bulk media and nanostructures. One of the effective and universal approaches to trigger the precession relies on changing magnetic anisotropy on the ultrafast time scale and, in general, can be realized in various media, e.g. metals, semiconductors and dielectrics.

In this talk we present an overview of the activities of the Ferroics Physics laboratory in the field of ultrafast magnetism and focus on controlling magnetic anisotropy of thin metallic and dielectric films by femtosecond laser pulses [5,6]. We discuss two mechanisms, both of which rely on absorption of laser pulse and fast increase of lattice temperature, which is a very general process, occurring in most of media subjected to femtosecond laser pulses. We demonstrate experimentally that the ultrafast lattice heating leads to change of magnetic anisotropy either directly, or via inverse magnetostriction. Also we show that the thin magnetic films grown on low-symmetry substrates exhibit response to the femtosecond optical excitation combining various processes, which can be used for a fine tuning of the parameters of the excited precession. As the objects media for these studies we've chosen dielectric magnetic garnets, the model media in magnonics, and metallic alloy Galfenol, the model magnetostrictive material. The studies were carried out using the magneto-optical pump-probe technique described in details elsewhere [4].

100-nm thick film of metallic alloy Galfenol $Fe_{0.81}Ga_{0.19}$ was grown on (311) GaAs substrate by magnetron sputtering. We show [5] that excitation of the film by femtosecond laser pulse launches the precession of magnetization which frequency, amplitude and initial phase can be controlled by changing the strength of the external magnetic field. While the field dependence of the first two parameters is trivial, the control of the initial phase of precession in a wide range of $0\text{-}90^{o}$ has been demonstrated in such kind of experiments for the first time, to the best of our

knowledge. Detailed study of the laser-induced precession allowed us to distinguish two mechanisms responsible for the excitation. The first one relies on ultrafast lattice heating and picoseconds change of magnetocrystalline anisotropy, and has been known from earlier studies of laser-induced magnetization precession in metals. The second mechanism relies on strain occurring due to lattice expansion, being a result of the heating. We show that the efficiency of these two mechanisms in the low symmetry Galfenol film changes when the external magnetic strength is tuned, which leads to the observed control of the initial phase of the excited precession by the field.

Triggering the magnetization precession via ultrafast change of the magnetic anisotropy, being a result of laser-induced lattice heating, has been well investigated in magnetic metals. However, the efficiency of this mechanism in thin magnetic dielectric films remains unclear. In order to investigate this issue we have studied the laser-induced magnetization dynamics in a 5-um thick single crystalline iron garnet $Y_3Fe_5O_{12}$ film grown on (210) gadolinium gallium garnet substrate by liquid phase epitaxy. Studies of the magnetization dynamics excited by femtosecond laser pulses [6] have shown that the precession of magnetization occurs via two distinct mechanisms. The first one is the ultrafast inverse Faraday effect (IFE), which is the well-known phenomenon in ultrafast magnetism of dielectrics [3,4]. However, along with the polarization dependent excitation of the precession, ascribed to IFE, we have also observed the polarization-independent excitation. Detailed study of this process allowed us to conclude that there is an ultrafast change of the growth-induced magnetic anisotropy induced by the femtosecond laser pulse. We argue that this process relies on ultrafast heating of the lattice. Importantly, the efficiencies of the precession excitation via IFE and via anisotropy change are comparable, but exhibit different dependences on the external magnetic field strength. This allows for tuning the parameters of the excited precession by changing magnetic field and laser pulse polarization.

In conclusion, we would like to stress that in both studies the low symmetry of the magnetic films allowed to realize the combined excitation of magnetization precession via different mechanisms. This opens a possibility of tuning the parameters of the excited precession, including its initial phase, by changing the exciting optical pulse properties or applied magnetic field. We beleave that such a flexibility of is interest for application in spintronics and magnonics.

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Kardakova Anna
Phd
Researcher

Energy relaxation in superconducting boron-doped diamond films

SCIENTIFIC ORGANIZATION

Moscow State Pedagogical University

ABSTRACT

The research is dedicated to the experimental study of the energy relaxation time of the electron system in thin boron-doped diamond films at low temperatures. The main results confirm that the energy relaxation time in the studied samples is due to the electron-phonon scattering time which is material- and temperature- dependent. The experimental results are important for the development of sensitive superconducting bolometers and resonator-based detectors for optical and infrared (THz) radiation.

KEYWORDS

Electron-phonon interaction, superconducting boron-doped diamond.

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation, contract No. 14.B25.31.0007.

SUMMARY

We report on our study of the relaxation time of the resistive superconducting state in single-crystalline boron-doped diamond films performed with the technique of amplitude-modulated absorption of (sub-) THz radiation. The films have a carrier density of about 2.5×10^{21} cm^{-3}, a critical temperature of about 2 K and a high normal-state resistivity ρ_n~1500 μΩ·cm. Our main result is that the slow electron-phonon relaxation time at low temperatures is governed by a T^{-2}-dependence with a value of 0.7 μs at T = 1.7 K. The high normal-state resistivity and remarkably slow electron-phonon relaxation confirm that superconducting boron-doped diamond films are a prospective material for ultrasensitive superconducting bolometers and resonator detectors.

A. Kardakova, A. Shishkin, A. Semenov, S. Ryabchun, J. Bousquet, D. Eon, B. Sacépé, Th. Klein, E. Bustarret, G. N. Goltsman, and T. M. Klapwijk, *Relaxation of the resistive superconducting state in superconducting boron-doped diamond*, Phys. Rev. B 93, 064506 (2016).

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Professor of Physics, Senior Researcher

Big Data processing at High Energy Physics experiments

SCIENTIFIC ORGANIZATION

Jozef Stefan Institute and University of Ljubljana

ABSTRACT

I present various aspects of the computing resource needs experiments in HEP, in particular at the Large Hadron Collider at CERN, have encountered so far and how this will evolve in the future when moving from LHC to HL-LHC ten years from now, as the already Exa-scale levels of data we are processing could increase by a further order of magnitude. The distributed computing environment has been a great success and the inclusion of new super-computing facilities for the future a big challenge, which we are successfully mastering with a considerable contribution from our Russian colleagues.

KEYWORDS

HEP, LHC, Computing, Super-Computers.

Khripunov Sergey
Engineer

Coherent population trapping resonance formation delay under dynamic excitation in 87Rb

SCIENTIFIC ORGANIZATION

Novosibirsk State University

ABSTRACT

Effect of electromagnetically-induced transparency delay generated by dynamic coherent population trapping (CPT) is poorly understood for today. In the current work we experimentally investigate the dependency of the delay upon different parameters. It was found out that the delay depends upon the modulation parameters of the frequency difference between two laser fields and doesn't depend upon relaxation properties of Rb vapor cell.

KEYWORDS

Coherent population trapping, atomic clock, dynamic excitation of an atomic system.

ACKNOWLEDGEMENTS

MESRF №2014/139 pr №825, RSCF №16-12-10147.

SUMMARY

Current work describes a new effect which consists in an appearance of a delay of an electromagnetically induced transparency under conditions of quick periodical excitation of a coherent population trapping resonance. The effect was discovered by our group during work with an atomic frequency standard. The work is a part of a research which aims to study properties of a CPT resonance under dynamic excitation. The work reports on results of experimental and theoretical researches of the dependency of phase delay upon the frequency of scanning near the CPT resonance.

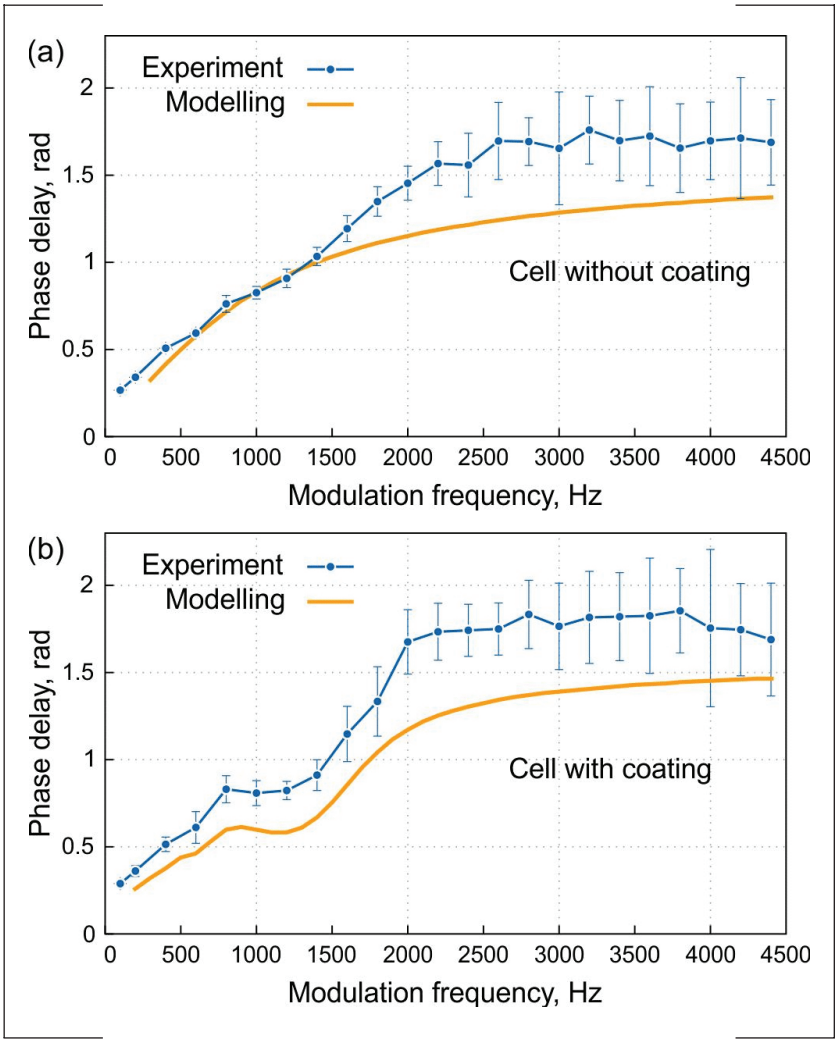

Fig. 1. Dependency of the phase delay of the CPT resonance excitation upon the frequency of modulation of the difference frequency of the bichromatic field components:
a) optical cell without an anti-relaxation coating or buffer gas,
b) optical cell with an anti-relaxation coating

Excitation of a coherent population trapping resonance is a result of an interaction between a three-level energy system and a bichromatic electromagnetic field. Performing a sinusoidal modulation of the frequency difference of components of the field leads to a periodical excitation of the resonance. When the modulation frequency is low, maximums of the transmittance curve are located at zeroes of the sinusoidal modulation signal. However, increasing of the modulation frequency leads to non-zero shift of locations of transmittance curve maximums relative to zeroes of modulation signal. *Phase delay* is a delay between a CPT resonance peak and zero of the modulation signal expressed by phase of the modulation signal.

We conducted an experimental study of the dependence of phase delay upon modulation frequency, results are following (Fig. 1) : the phase delay value increases with the increase of modulation frequency linearly (modulation frequency less than 2 kHz) and reaches the saturation level of 1.7 ± 0.3 rad (at 2 kHz). In order to examine dependency of the phase delay upon relaxation properties of an active media, we conducted

experiments for cases of an optical cell without an anti-relaxation coating or buffer gas (Fig. 1, (a)) and for a cell with an anti-relaxation coating (Fig. 2, (b)). Experimental results showed no dependency upon this factor. Furthermore, a theoretical study was conducted. It consisted in a numerical solution of differential equations on the elements of the density matrix of a three-level energy system. Using the numerical solution, a similar dependency was obtained. The result of modeling correspond experimental results, but there is a numerical difference (saturation value 1.4 ± 0.02 rad for the theoretical results) that can be explained by the simplicity of the mathematical model used for theoretical study.

This work reports on a new effect which consists in an appearance of a coherent population trapping resonance formation delay under circumstances of a dynamic excitation. This effect was discovered by our group during work with a frequency atomic standard. The effect has a critical impact on a feedback system of the standard.

Khromov Alexander
PhD student
Engineer

Search for coherent elastic neutrino-nucleus scattering with RED-100 detector

SCIENTIFIC ORGANIZATION

National Research Nuclear University MEPhI

ABSTRACT

The RED-100 (Russian Emission Detector) is constructed for search of coherent elastic neutrino-nucleus scattering (CEvNS) off atomic nuclei. This fundamental process was predicted several decades ago by the Standard Model of electroweak interactions but has not been discovered yet. The RED-100 is an emission two-phase xenon detector containing ~200 kg of liquid Xe (~ 100 kg in a fiducial volume). The detector description is given covering principle of operation, technical details and current status. Future plans for detector deployment at the experimental site are presented.

KEYWORDS

Neutrino physics, emission detector, liquid xenon, rare events search, low-background experiment.

SUMMARY

The RED100 detector is built to search for coherent elastic neutrino-nucleus scattering (CEvNS) off atomic nuclei. This process was predicted by the Standard Model but has never been observed yet. The RED-100 is an emission two-phase xenon detector containing ~200 kg of liquid Xe (~ 100 kg in a fiducial volume). The RED100 experimental setup consists of several systems that provide stable and effective operation. These systems are the detector itself located inside a shielding, cryogenics, purification, light collection, electronics and data acquisition. The detector principle of operation and design are described.The current status of the RED100 detector is discussed as well. Future plans for the detector installation at a neutrino source are given.

Krasnopolsky Vladimir
Doctor of physics and math
Research Professor

Atmospheres of Mars, Venus, and Titan

SCIENTIFIC ORGANIZATION

Catholic University of America

ABSTRACT

Our grant 11.G34.31.0074 was extended for two years (2014 and 2015). We continued in that period (1) analysis and interpretation of observations from Mars Express and Venus Express orbiters, (2) ground-based high-resolution spectroscopy of Mars and Venus, (3) three-dimensional modeling of circulation in the atmospheres of Mars, Venus, and Titan and photochemical modeling of those atmospheres, and (4) preparation of the Atmospheric Chemistry Suite for the ExoMars orbiter mission, design and manufacturing of new instruments for planetary research.

KEYWORDS

Mars; Venus; Titan; atmospheres; spectroscopy; photochemistry.

ACKNOWLEDGEMENTS

This work was supported by grant 11.G34.31.0074 from Ministry of Science and Educations of Russian Federation.

SUMMARY

Our grant 11.G34.31.0074 was extended for two years (2014 and 2015). We continued in that period (1) analysis and interpretation of observations from Mars Express and Venus Express orbiters, (2) ground-based high-resolution spectroscopy of Mars and Venus, (3) three-dimensional modeling of circulation in the atmospheres of Mars, Venus, and Titan and photochemical modeling of those atmospheres, and (4) preparation of the Atmospheric Chemistry Suite for the ExoMars orbiter mission, design and manufacturing of new instruments for planetary research.

Kusmartsev Fedor
PhD
Professor of Condensed Matter

Thorny Road to Topological Insulators and Weyl Semimetals

SCIENTIFIC ORGANIZATION

Loughborough University

ABSTRACT

The recent discovery of the novel materials - Weyl semimetals in 2015 completely changed our views on matter. I will describe a thorny historical way which lead to this discovery. I will discuss the main physical properties of Weyl semimetals and compare them with various topological insulators as well as two- dimensional crystals such as graphene, silicene, germanene and compare them with those of poly- acetylene. The issues associated with Fermi arc and chiral anomaly in Weyl semimetals and simplest devices made of them will be described.

KEYWORDS

Topological Insulators, Weyl semimetals, snake states, two-dimesional crystals.

SUMMARY

The recent discovery of the novel materials - Weyl semimetals in 2015 completely changed our views on matter. I will describe a thorny historical way which lead to this discovery. I will discuss the main physical properties of Weyl semimetals and compare them with various topological insulators as well as two- dimensional crystals such as graphene, silicene, germanene and compare them with those of poly-acetylene. We comment on the origin of their buckled two-dimensional shape and draw their analogy with the Peierls distortions in polyacetylene. We also address

the issues created by the Mermin-Wagner theorem prohibiting the existence of strictly two-dimensional crystals. Then we describe the main ideas which led to the discovery of topological insulators and Weyl semimetals and comment on a formation of Majorana fermions in these systems. We describe some of the outstanding electronic properties originate due to the breaking of fundamental symmetries as well as an existence of the Dirac and Weyl gapless spectra. The issues associated with Fermi arc in Weyl semimetals will be described. I will also compare properties of simplest devices made of Weyl semimetals and Dirac materials. Analogies and differences between Dirac materials, Weyl semimetals and optics will be also discussed.

Kuzmin Leonid
Dr.Sci.
Professor

Megagrant on Cosmology and European Competition

SCIENTIFIC ORGANIZATION

Chalmers University of Technology

ABSTRACT

For investigation of the Cosmic Microwave Background we developed the Cold-Electron Bolometers (CEB) insensitive to Cosmic Rays. We are invited to develop detectors for the OLIMPO and LSPE experiments devoted to Syunyaev-Zel'dovich effect. We are developing multichroic systems based on concept of Resonance CEB invented by Swedish-Russian collaboration for the European COrE space mission. CEB is the only European concept daring to compete with dominating of American concepts. However, these opportunities to go to the international level do not find proper support of MON.

SUMMARY

The Cosmic Microwave Background is a powerful probe for the primordial universe and the high energy physics; through the SZ effect it can provide information about the physics of galaxy clusters. The recent joined analysis of BICEP2 experiment and Planck satellite rejected a B-modes detection by BICEP2, demonstrating the stringent necessity of **multifrequency CMB experiments** to correct the observations from the dust contributions. The Planck mission produced accurate maps of the sky with performances close to be limited by Cosmic Rays (CRs). This demonstrated the **mandatory development of bolometers less affected by the interaction with CRs.**

We propose the development of **the Cold-Electron Bolometers (CEBs) based on direct electron cooling of the absorber by SIN tunnel junctions.**

First tests have provided high level of the immunity of the CEBs chips. Further tests, with a larger statistics, would strongly confirm these results. **CEBs** represent **a promising alternative to commonly used TES detectors which suffer for CRs sensitivity** and other issues (saturation problems, sensitivity to magnetic fields...).

We plan to assess the level of immunity of CEBs towards CRs; optimized CEBs arrays will be developed for studying the interactions with radioactive sources, providing a stringent result about their level of immunity.

In the second part we will develop detectors for the OLIMPO experiment, devoted to Syunyaev-Zel'dovich spectro-photometric observations of galaxy clusters.

In the third part we will develop detectors for the LSPE experiment devoted to study of the primordial universe and the properties of the interstellar dust.

In the field of multifrequency systems we are developing multichroic systems based on two concepts: **Resonance Cold-Electron Bolometer (RCEB)** and **Seashell Slot Antenna**. Both concepts were invented by Swedish-Russian collaboration and are developed by ESA (European Space Agency) consortium.

The Cosmic Microwave Background (CMB) is the radiation emitted when the universe was about 380000 years old. Its polarized component, B-modes, is a powerful probe for understanding the primordial universe and the high energy physics. Moreover, the CMB interaction with intracluster gas of galaxy clusters (the so called SZ effect) can provide information about the physics of galaxy clusters

itself. Recent Planck and BICEP2 experiments only improved upper limits on B-modes. Moreover, the Planck mission was close to be limited by interactions between its detectors and Cosmic Rays (CRs). These demonstrated the necessity of developing multi-frequency experiments to correct B-modes observations from astrophysical contaminant signals with detectors immune to CRs.

We propose the development of the Cold-Electron Bolometers (CEBs), based on direct electron cooling of the absorber by Superconductor-Insulator-Normal tunnel junctions. The smaller volume of absorber makes CEBs intrinsically insensitive to CRs with respect to commonly used bolometers. In this aim, we will fabricate CEBs arrays optimized to strongly assess their level of immunity towards CRs. We propose to develop CEBs for the Italian balloon borne experiments OLIMPO and LSPE, devoted to multifrequency observations of the SZ effect and B-modes, respectively.

CEB is considered as the third concept for a new European COrE (Cosmic Origias aExplorer) space mission after TES and KID American concept. CEB developed by Swedish –Russian collaboration is the only European concept osmelivshayasya to compeate with dominating of American concepts. It looks that we have a unique chance to participate and really contribute to international development of Cosmology. However, our authorities do not support this participation. This opportunity to go to the international level declared in goals of Megagrants really does not find any support of authorities. Besides that, a very low level of support money is delayed by half a year or more. It creates very difficult situation with support of scientists, especially young scientists. We can accept that MON has problems with money as in whole in Russia but delay with payment is fully responsibility of the MON.

Lagoudakis Pavlos
PhD
Professor

Quantum Technologies

SCIENTIFIC ORGANIZATION

University of Southampton

ABSTRACT

Finding the ground state of physical systems is the natural quantum analogue of classical constraint satisfaction problems that are mapped into various optimization problems in technology and life sciences. Most of these problems belong to the non-deterministic polynomial time (NP)-complete or NP-hard complexity classes and cannot be solved efficiently using classical digital computers. Here, I will present recent advances on quantum simulations of Ising chains and 2-D frustrated classical magnetism utilising polariton graphs.

Keywords

Polaritons AND quantum AND simulators.

Summary

Quantum Simulations with Polariton Graphs

Prof Pavlos Lagoudakis

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Finding the ground state of physical systems is the natural quantum analogue of classical constraint satisfaction problems that are mapped into various optimization problems in technology and life sciences. Most of these problems belong to the non-deterministic polynomial time (NP)-complete or NP-hard complexity classes and cannot be solved efficiently using classical digital computers. By calculating the ground state energies of a physical system of a given complexity class one can solve any problem in the same complexity class according to the Cook-Levin theorem [1-3]. It has been established that quantum generalisation of constraint

satisfaction problems is provided by the k-local Hamiltonian problem [4], which is quantum Merlin-Arthur (QMA)-complete for k≥2 [5], where QMA is the quantum analogue of NP. For QMA-complete (NP-complete) problems there are no classical or quantum polynomial-time algorithms to solve them. One way to tackle such computationally intractable problems is to construct a controllable quantum system - a quantum simulator -- for which the calculation of the ground state provides the solution for one and thus all of the NP-complete or NP-hard problems. Apart from potentially solving classical NP-complete or NP-hard problems a major motivation for constructing a quantum simulator for the k-local Hamiltonian problem is in simulating quantum mechanics in large condensed-matter, cosmological, high-energy, atomic, and other systems described in terms of k-local Hamiltonians with restricted types of interactions. Here, I will present recent advances on quantum simulations of 1-D Ising chains and 2-D frustrated classical magnetism utilising polariton graphs.

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Lapin Vicktor

Junior researcher

Temporal and spectral compression of pulses in fibers with a running refractive index wave

SCIENTIFIC ORGANIZATION

Technological Research Institute of Ulyanovsk State University

ABSTRACT

For pulses propagating in fibers with a running refractive index wave, the pulse power could be drastically increased due to decrease of the pulse duration. We report temporal and spectral compression of the pulses and conditions for formation of soliton-like chirped pulses in nonlinear fibers with a running refractive index wave. We demonstrate possibility of 100- fold compression of the wave packets propagating in media with a running refractive index wave (down to subpicosecond durations).

Keywords

Ultra short optical pulses, nonlinearity, running refractive index wave, sub-picosecond pulses, modulation instability, wave packets, nonlinear fibers, temporal and spectral compression of the pulses.

Acknowledgements

This work was supported by the Ministry of Education and Science of the Russian Federation (Project No.14.Z50.31.0015).

Summary

It is known that when a light pulse propagates through anoptical fibre, in which a running refractive-index wave(RRIW) is generated, one can observe the effects that are absent both in homogeneous fibres and in fibres with a static inhomogeneity or periodicity. The authors of Refs studied the effects related to a change in polarisation and carrier frequency offset of quasi-monochromatic wave packets under the RRIW influence. Pulsed regimes of light propagation in optical fibres with a RRIW

are characterised by a several-fold increase in the pulse power with a corresponding reduction of its duration. However, despite the abovesaid, current publications (except for a relatively small number of papers; see e.g.) lack a detailed examination of the possibility of the control of the frequency modulation rate and the spectral width of pulses interacting with a RRIW.

In this paper we investigate the conditions for temporal and spectral compression of frequency-modulated (FM) Gaussian pulses propagating in a fibre with a RRIW. It is shown that such a fibre can be characterised by a strong pulse frequency modulation at a constant linear velocity. This fact can be used for the subsequent strong spectral or temporal compression. We present analytical expressions for the dependences of duration, spectral width and initial rate of frequency modulation of a (chirp) pulse on the distance travelled along the fibre. Based on the numerical analysis we have studied the behaviour of these characteristics by changing the coefficient of the refractive-index modulation and other parameters of the RRIW. To modulate pulses with their subsequent compression in dispersing elements (optical fibres or diffraction gratings) one can use not only fibres, but also planar structures.

The analysis performed in this paper shows that optical fibres with a RRIW synchronised (by the propagation velocity) with the pulse launched into the optical fibre can be used for strong frequency modulation of the corresponding pulses at a small (less than 10 cm) length of the waveguide modulator. In this case, even at this length of the fibre, one can obtain a considerable spectral broadening of the pulse (by 1 – 3 orders of magnitude, up to $\Delta\omega = 10^{14}\ \mathrm{s}^{-1}$ inclusive) at a virtually ideal preservation of the chirp linearity.

The latter circumstance, in turn, makes possible the subsequent strong pulse compression (temporary compression) by 1 – 3 orders up to subpicosecond and femtosecond values (in the optical range). On the other hand, the corresponding waveguide modulators (such as fibre and planar ones) can be used for the spectral compression of initially frequency-modulated broadband pulses.

The set of appropriate techniques (both spectral and temporal compression) can be successfully used in CPA for amplification of frequency-modulated pulses in the highpower subpicosecond and femtosecond laser systems.

Limonov Mikhail
Prof
Principal research scientist

Phase transition from photonic crystals to all-dielectric metamaterials

SCIENTIFIC ORGANIZATION

ITMO University and Ioffe Institute

ABSTRACT

Photonic crystals and all-dielectric metamaterials represent two different classes of artificial structures often composed of similar based elements. The question is how to distinguish these two types of periodic structures when their parameters (lattice constant and dielectric permittivity) vary continuously. We analyzed a transition between photonic crystals and dielectric metamaterials and introduce the concept of a phase diagram.

KEYWORDS

Photonic crystals, metamaterials, phase transition, phase diagram.

ACKNOWLEDGEMENTS

This work was supported by the Russian Foundation for Basic Research (No. 15-02-07529).

SUMMARY

We considered two different scenarios for the transition of a two-dimensional square lattice of dielectric rods from photonic crystals (PhC) to all-dielectric metamaterials (MM) [1]. The first scenario occurs when the lattice constant *a* decreases in comparison with the fixed radius of rods *r* and dielectric permittivity

ε remains constant. This transformation leads to an increase of the filling ratio *r/a* and it makes possible the homogenization of the periodic dielectric structure with the negative effective permeability (μ<0) at higher values of ε. The second scenario occurs when the dielectric permittivity of rods ε varies in a fixed square lattice. This transformation leads to an increase of the Mie scattering wavelength, and it can also provide the conditions for the homogenization approach with negative μ.

We show that a PhC structure transforms into a MM when the Mie gap opens up below the lowest Bragg bandgap. Our theoretical approach was confirmed by microwave experiments for a metacrystal composed of tubes filled with heated water. We also introduced the concept of a phase diagram in the permittivity-filling ratio plane. The boundaries of the MM phase have been obtained theoretically and confirmed experimentally. On the basis of the proposed approach, one can obtain different PhC–MM phase diagrams by altering the dimension, symmetry, composition, size and geometry of the structural elements within a unit cell. This analysis yields deep insight into the properties of periodic structures, and provides a useful tool for designing different classes of electromagnetic materials with variable parameters.

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Candidate Of Science
Engineer

The Relation Between The Elastic And Electronic Structure Properties Of Niobium Under Ultrahigh Pressures

SCIENTIFIC ORGANIZATION

Materials Modeling and Development Laboratory, National University Of Science and Technology «MISIS»

ABSTRACT

We present qualitatively new picture of the relation of electronic structure and elastic properties in pure niobium. Carefull theoretical study were performed to figure out the impact of electronic topological transition (ETT) on the character of stress-strain relations in the material. A peculiarity of the elastic properties of Nb is clearly observed in the pressure range of 0-100 GPa. The role of the electronic structure modification upon deformation in this effect can be clearly distinguished. We belive that obtained results may change the understanding of elasticity of solids.

Keywords

Ab initio modeling, solids, elasticity, electronic structure.

Acknowledgements

The support from the Grant of Ministry of Education and Science of the Russian Federation (Grant No. 14.Y26.31.0005) is gratefully acknowledged. Calculations were performed on the Computational Cluster of NUST MISIS “Cherry”.

Summary

The focus of this work are the effects of electronic structure on the elastic properties of solids at ultrahigh pressures. It is known, that electronic topological transitions, which take place under extreme compressions are responsible for many unique effects. We chose niobium as the object of study, since the transition metals are the usual material for samples in groundbreaking experimental works in the field of static high pressure techniques. At the same time the 5-th group transition metals (V, Nb, Ta) demonstrate an outstanding combination of properties as well as interesting behavior under pressure. For example, vanadium is known to have phase transition to low symmetry phase at the pressure of ~70 GPa. The presence of electronic topological transition in both vanadium and niobium are well known from the literature, at the same time, intense studies are usually only dedicated to the former.

We present qualitatively new picture of the relation of electronic structure and elastic properties in pure niobium. Careful *ab initio* calculations were performed to figure out the impact of electronic topological transition (ETT) on the character of stress-strain relations in the material. A peculiarity of the elastic properties of Nb is clearly observed in the pressure range of 0-100 GPa. The range of strains in which the Hook's low holds is shrinking upon the approach to the ETT at high pressure, and effectively vanishes at the ETT. The role of the electronic structure modification upon deformation in this effect can be clearly distinguished. The mechanism of this subtle, but explicilty observed relation is discussed. The fundamental nature of the phenomena points on the possibility of such effects in other metallic systems.

ADDITIONAL INFORMATION

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Lyubomirskiy Mikhail
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Postdoc

Hard X-ray in-line interferometers fabricated by Si planar technologies

SCIENTIFIC ORGANIZATION

DESY Photon Science

ABSTRACT

The modern microfabrication technologies allowed profiling of Si crystals to a significant depth with a high quality of vertical sidewalls offering unique opportunities for manufacturing of X-ray interferometers based on compound refractive lenses (CRL) and reflecting mirrors. The proposed interferometers can be applied for coherence and optics characterisation, surface metrology in the energy range 5-100 keV. The high contrast of the tunable interference pattern can be used for new type of moiré radiography and standing wave techniques.

KEYWORDS

Synchrotron radiation, X-ray optics, interferometer, refractive lenses, mirrors.

ACKNOWLEDGEMENTS

The work was supported by the Ministry of Science and Education of Russian Federation grant № 14.Y26.31.0002.

SUMMARY

The modern microfabrication technologies allowed profiling of Si crystals to a significant depth with a high quality of vertical sidewalls offering unique opportunities such manufacturing of X-ray optical elements like planar compound refractive lenses (CRL) and bilens interferometers [1, 2]. The CRL based bilens interferometer consists of two parallel lens arrays which under coherent illumination produces the interference pattern i.e. standing wave with a variable period ranging from tens of nanometers to tens of micrometers, depending on the observation distance.

Recently, in order to expand bilens beam acceptance, we have proposed a multilens system [3]. The interference field produced by the multilens system, in comparison with the bilens, has a more rich longitudinal structure and may be described by the Talbot imaging formalism. The increase of the beam acceptance raises an intensity and a contrast of the interference pattern leading interference maxima narrowing which is confirmed by the experimental studies [3]. The large interferometer "aperture" gives higher sensitivity and precision for characterization of the beamline optics.

Another promising option offered by the microfabrication technologies is the ability to create reflection-based systems, where sidewalls of the etched structures can

be used as reflecting mirrors: two parallel mirrors represent a micro-mirror interferometer [4]. Experimental tests showed that the interference pattern produced by such interferometers is sensitive to a roughness of the etched surface.

The proposed interferometers can be applied for coherence and optics characterisation, surface metrology in the energy range 5-100 keV. Finally, high contrast of the tunable interference pattern can be used for new type of moiré radiography and standing wave techniques. The strong advantage of Si planar technologies is the ability to create integrated optical systems on one chip consisting of refractive lenses, lens- and mirror-based interferometers. A scanning electron microscope (SEM) image of such chip is disposed in Fig. 1.

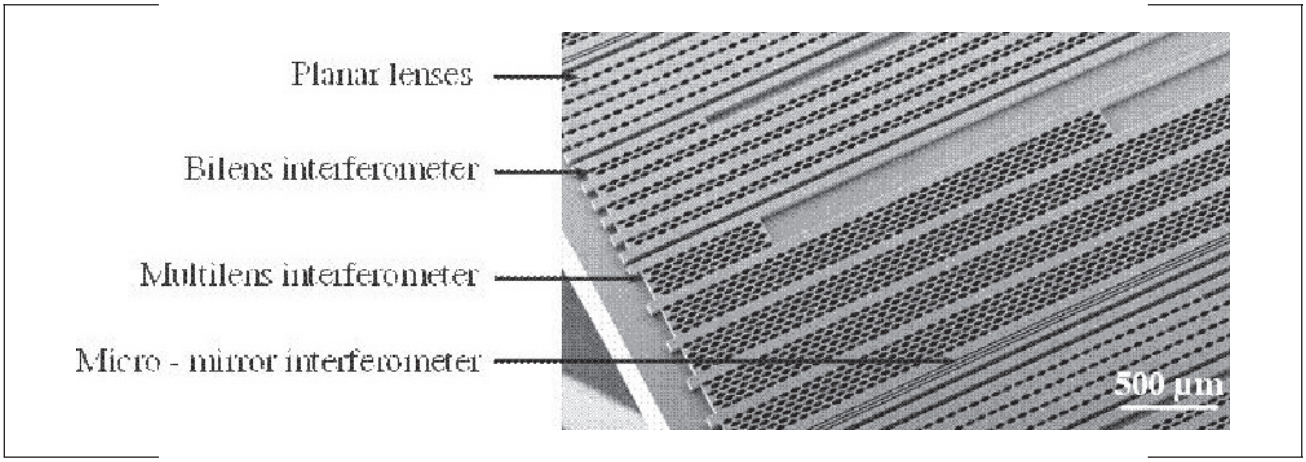

Fig. 1. SEM image of a Si chip containing different X-ray optical elements.

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ADDITIONAL INFORMATION

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Plasma Surface Interactions and Plasma Technologies

SCIENTIFIC ORGANIZATION

National Research Nuclear University MEPhI

ABSTRACT

The Laboratory of “Plasma Surface Interactions and Plasma Technologies” was established at MEPhI in 2014. This is a 3+2 years project of the RF’s Government. In this talk we present main results of our work for past 2 years.

KEYWORDS

Plasma, tokamak, technology, first wall.

ACKNOWLEDGEMENTS

This project is supported by Russian Ministry of Education and science, mega-grant 14.Y26.31.0008.

SUMMARY

The Laboratory of "Plasma Surface Interactions and Plasma Technologies" was established at MEPhI in 2014. This is a 3+2 years project of the RF's Government. The main official research foci of the Lab are plasma-material interactions in fusion devices, including: trapping and transport of hydrogenic and He species in material, surface morphology and material properties modifications, development of new armor materials for the first wall. Technological part includes research of material hardening and fatigue modification, improvements of electric properties of materials used in capacitors.

The Lab has both experimental and theoretical parts which work in a close collaboration providing cross-fertilization and unified effort in research. We also collaborate with other research institutions both domestic and international.

To facilitate the research activity the Lab will the following hardware has been acquired: computer cluster for computationally demanding simulations (including DFT, MD, PIC, MC, BOUT++, UEDGE, etc.); tools for cross section of samples for SEM observations; Optical microscope for metallography; Optical pyrometer (2000°C, 0.2 mm spatial resolution) for registration of the temperature maps of samples exposed in plasma; Quadroupole mass spectrometer with He – D2 resolution.

To have the outside opinion on the directions and quality of our work and to promote our future achievements, the Lab's Scientific Advisory Board was formed. It includes: Dr. Richard Pitts, IO (Leader of Divertor and Plasma-Wall Interactions Section), Dr. Russ Doerner, UCSD (Head of the PISCES Lab), Prof. Dave Ruzic, UIUC (Director of Center for Plasma-Material interactions), Prof. Sungho Jin, UCSD (Director of Materials Science and Engineering Program), Prof. Nariyasu Ohno, Nagoya U. (Head of the NAGDISS Lab).

Two years of the Lab functioning gave new interesting results in physics of plasma-surface interactions, having as fundamental as practical applications. The main topics of our work were research of hydrogen isotopes behavior in solids, investigation of erosion of plasma-facing components in tokamaks, developing of new ways to produce protecting coatings for different materials, and many others. Our team has sufficiently grew up owing to both young guys and experienced researchers who join the Lab being interested by physical problems within our scope, and possibilities which we are able to provide to our employees. Results of our work were published in leading scientific journals and were presented at several international conferences.

ADDITIONAL INFORMATION

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Enantioselective interaction of chiral semiconductor nanocrystals and tumor cells

SCIENTIFIC ORGANIZATION

ITMO University

ABSTRACT

The aim of study was to investigate the enantioselective interaction of semiconductor nanocrystals of different shapes with living tumor cells. Using methods of confocal fluorescence microscopy and FLIM we investigated optical properties, cellular uptake and cytotoxicity of chiral nanocrystals against A-549 and Ehrlich Ascite carcinoma cell lines. We demonstrated evident enantioselective cellular uptake and cytotoxicity of chiral nanocrystals while the intracellular optical properties of nanocrystals did not depend on their chirality.

KEYWORDS

Quantum dots, quantum rods, quantum tetra-pods, cytotoxicity, cellular uptake, fluorescence spectroscopy, FLIM.

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation (Projects 14.B25.31.0002, 3.109.2014/K).

SUMMARY

Chirality is a common property of the most part of active biological molecules that provide their stereospecific interactions with environment. Many properties such as the ability to penetrate into cells, enzymatic activity and toxicity are strongly dependent on chirality of substances.[1]

A creation of man-made chiral inorganic structures is a hot trend in nanotechnology today. An acquisition by nanostructure chiral properties should lead to significant changing in their interactions with biomolecules. It opens new possibilities to realize stereospecific interactions of nanostructures in biological environment.[2]

Semiconductor nanocrystals (NCs)[3] is a vivid specimen of man-made inorganic nanoparticles that can be widely used in many fields of biological studies. [4] Recent studies demonstrated for the first time the induction of chiroptical activity in NCs.[2-5] NC s are able to obtain chirality as the result of attaching the chiral molecules to the NC surface.[2]

To fully understand the interactions between NC s and living cells in order to develop nontoxic and biocompatible NC s for clinical use the impact on living organisms of the chirality of NC s should be investigated. Different chiral properties of NC s may determine their ability to interact with other biomolecules and thereby modulate a range of downstream processes in living cells. In[5] was demonstrated differential NC cell toxicity associated with the chirality of glutathione coating of CdTe quantum dots (QDs). QDs coated with D-glutathione, the nonbiologically active form of glutathione, showed less cytotoxicity than L-glutathione-coated QDs.

The aim of study was to investigate the enantioselective interaction of semiconductor nanocrystals of different shapes and living tumor cells. Using methods of confocal fluorescence microscopy and FLIM we investigated optical properties, cellular uptake and cytotoxicity of chiral nanocrystals against A-549 and Ehrlich Ascite carcinoma cell lines.

Hydrophobic trioctylphosphine oxide (TOPO) capped CdSe/ZnS spherical quantum dots, dots in rods and dots in tetrapods were prepared according to methods described in.[6] Chiral NCs were obtained from hydrophobic CdSe/ZnS NCs by the method of post-synthesis ligand exchange using D- and L-cysteine (Cys) as chiral ligands.

Circular dichroism spectra of the D- and L-cysteine capped NC demonstrated a pronounced antiphase optical dichroism signal in the spectral region of intrinsic NC absorption

Cell toxicity and intracellular accumulation of NCs were investigated on A-549 and Ehrlich Ascite carcinoma cells by high content screening and confocal PL microscopy respectively.

Optical properties of NCs inside A-549 and Ehrlich Ascite carcinoma cells were studied by confocal PL microscopy and time-resolved PL microscopy to obtain PL intensity and PL lifetimes data of NCs inside cells.

It was shown that chirality of NCs did not influence on their optical characteristics inside cells, but had crucial role in the NC cytotoxicity and cellular uptake. It was demonstrated that L-Cys NCs had higher cellular accumulation in the case of Ehrlich Ascite carcinoma cells while D-Cys NCs were more biologically active in A-549 cells. Cytotoxicity of chiral quantum dots against Ehrlich Ascite carcinoma cells did not exceed 10% in the concentration region 1–20 μmol L–1 of QDs. In this case, L-Cys QDs had slightly higher cytotoxicity than D-Cys QDs. However, D-Cys NCs had more pronounced cytotoxicity than L-Cys NCs against A-549 cells. The establishment of exact mechanisms of NP biological effects is our ongoing research.

We believe that this finding may lay the groundwork for novel approaches to controlling the biological properties and behavior of man-made chiral nanomaterials in living cells.

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The impact of electron correlations on the energetics and stability of silicon nanoclusters

SCIENTIFIC ORGANIZATION

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ABSTRACT

Prediction of stable nanocluster structure is often hampered by the existence of many isomer configurations. This fact attaches additional importance to many-electron effects beyond DFT, because their contributions can change a subtle energy order of competitive structures. We consider the energetics of silicon nanoclusters Si10H2n (0< n <11). Our calculations performed with DFT, hybrid functionals and Hartree-Fock (HF) methods, as well as by the GW approximation (GWA), confirm a considerable sensitivity of isomer energy ordering to many-electron effects.

SUMMARY

The first-principles prediction of stable nanocluster structure is often hampered by the existence of many isomer configurations with energies close to the ground state. This fact attaches additional importance to many-electron effects beyond density functional theory (DFT), because their contributions can change a subtle energy order of competitive structures. To analyze this problem, we consider, as an example, the energetics of silicon nanoclusters passivated by hydrogen Si10H2n (0< n <11), where passivation changes the structure from compact to loosely packed and branched. Our calculations performed with DFT, hybrid functionals and Hartree-Fock (HF) methods, as well as by the GW approximation (GWA), confirm a considerable sensitivity of isomer energy ordering to many-electron effects.

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Near-Field Scanning Magneto-Optical Spectroscopy of Wigner Molecules

SCIENTIFIC ORGANIZATION

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ABSTRACT

We study emission spectra of single self-organized InP/GaInP QDs (sizes 100-200 nm) using high-spatial-resolution, low-temperature (5K) near-field scanning optical microscope (NSOM) operating at magnetic field strength B=0-10T. We observed vibronic-type shake-up structure of single electron QDs manifesting formation of two electron (2e) molecule in photo-excited state and we measure molecular bond length to be 40-140 nm. We observed dissosiation of charged exciton complexes on molecules induced by quantum confinement and magnetic field.

KEYWORDS

Nano-optics, spintronics, quantum dots, strongly correletaed electron systems.

ACKNOWLEDGEMENTS

This work has been supported by Ministry of the Education and Science of the Russian Federation (contract № 14.Z50.31.0021, 7th april 2014).

SUMMARY

Introduction

Few-electrons moving in a weak confinement potential can be localized and spatially ordered (crystallized) forming, so-called, electronic or Wigner molecule (WM). The possibility of such crystallization in infinite systems was predicted by Wigner in 1934 [1] and it occurs when the energy of Coulomb interaction between the electrons exceeds their kinetic energy. Theory predicts that for finite, quantum confined systems a transition from droplet to molecular phase is gradual with increase of the Coulomb to kinetic energy ratio, which is described by Wigner-Seitz radius $r_S=1/[a^*_B(p\cdot n)^{0.5}]$, where n is electron density and a^*_B is Bohr radius. Theory also predicts, that spatial ordering starts develop at $r_S>2$, and full localization in two-dimensional parabolic potential is realized at $r_S>100$, when charged particles can be considered as point classical charges [2]. Most of the experiments were performed for two electron (2e) WMs structures in epitaxial InSb nanowires [3], ultra-clean carbon nanotubes [4] and nano-fabricated GaAs/AlGaAs quantum dots (QDs) defined laterally [5] or vertically [6,7]. These systems were measured mainly using single-electron tunneling spectroscopy and provide parabolic confinement energy $\hbar w_0$=7.8-1.6 meV and r_S ~2 near the onset of the WM formation.

Here we study the formation of 2e-WMs in emission spectra of self-organized InP/GaInP QDs providing r_S up to 5. We used measurements of magnetic-field-induce shifts to distinguish emission of 2e-WM formed in photo-excited state from singly charged exciton (trion). We also observed magnetic-field-induced molecular-droplet transition for two electron dot, having doubly charge exiton (tetron) in photoexcited state at zero magnetic field.

Experimental details

The samples we grown by metal-organic chemical vapor deposition (MOCVD) in a horizontal AIX200/4 reactor under 100 mbar pressure at temperature 725 ^{O}C. The sample structure was as follows: 500 μm (100) GaAs substrate misoriented by 2^{O} towards the [110] direction, 50 nm thick GaAs buffer layer, 50 nm $Ga_{0.52}In_{0.48}P$ latticed matched to the GaAs, seven monolayers of InP to form the quantum dots, and finally 60 nm GaInP cap layer.

The quantum dot size, size distribution and composition were determined using an FEI Titan 80-300 transmission electron microscope (TEM). The sample preparation was done using focused ion beams.

Electron accumulation was detected by negative degree of circular polarization of emission of QD ensemble [8]. The measurements were carried out under non-resonant continuous-wave excitation using 632.8 nm line of He-Ne. Samples were placed in closed cycle helium cryostat with temperature~10 K. Helicity of light

in the excitation channel was alternated in sign at a frequency of 26 kHz, using photo-elastic quartz modulator. Quarter-wave plate followed by linear polarizer in the detection channel were used as a circular-polarization analyzer. Luminescence was dispersed by double monochromator and detected with photomultiplier tube. The degree of circular polarization , where I++,I-+ is intensity of σ+ luminescence under σ+, σ- excitation.

Single dot magneto-photoluminescence was measure using cryo near-field scanning optical microscope operating at 10 K and magnetic fields up to 10 T. We used tapered fiber probes coated by Al, having aperture size ~100 nm in collection-illumination mode [9]. The spectra were excited by the 514.5 nm Ar-laser line and measured using a CCD detector together with a 280 mm focal length monochromator. The excitation power was ~5 mW, which provided power density ~0.5 W/cm^2. The spectral resolution of the system is 0.2–0.4 meV. For near-field (NF) imaging we scan the tip across sample surface with the step 100 nm, measured spectra at each step and then generated emission intensity maps for given energy.

Calculation models

In the weak confinement regime charged excitonic complexes can be approximated as point-like particles and their single particle spectrum is described by Fock-Darwin (FD) Hamiltonian with corresponding parabolic frequency. The emission energy of trion (TR) is $E_{tr}=E_0+\hbar[w_{tr}-w_e(2k+1)]$, where E_0 is free 2D TR energy, $w_{tr}(w_e)$ are parabolic frequency of trion(electron), k is radial number of electron left in final state. Since $w_{tr}<w_e$, $E_{tr}(B)-E_{tr}(0)<0$, i.e. main PL peak (<0|0>-transition) has a paramagnetic shift, and, since w_{tr}not equal w_e, weak shake-up, <0|k>-transitions are activated [10]. Similar is valid for tetron (TE). For WM the electrons in photoexcited state are shifted from the position of electron in ground by half of molecular bond length d_0 and thus <k|0>-transitions is activated similar to that of stretching vibrations in diatomic molecules [11]. The intensities of <k|0>-transitions can thus be evaluated by Frank-Condon factors $F_k=\exp(-S)*S^k/k!$, were S is Stokes shift $S= m_e w_0^2(d_0/2)^2/2\hbar w_0$ and m_e is electron effective mass. The magnetic field shift of <0|0>-transition is $[E_{2e,r.m.}(B)+E_{C,2e}(B)]+E_h(B)+E_{C,2eh}(B)$,where $E_{2e,r.m.}(B)/ E_h(B)$ is FD energy of relative electron/hole motion and two rest terms are Coulomb interaction energies. The term in squire brackets was analyzed in [12] and represent difference between interacting and non-interacting two electrons. We calculated this terms and used it to estimate $E_{C,2eh}$ from experimental data.

For calculations of energy transitions of InP/GaInP QDs we used COMSOL Multiphysics 5.1 program and material parameters from Ref. [13]

Structural data versus near-field imaging and spectroscopy

The dot lateral size, D, measured using TEM is varied from 80 to 220 nm. Using energy dispersive X-ray analysis of cross section TEM specimens we reveal intermixing resulted in incorporation of ~20% Ga in QDs. The dots are lens shaped having heights h=5 and 20 nm. These heights were also observed by us using atomic force microscopy of uncapped dots and was previously reported in Refs [14-17]. In low-temperature ensemble PL spectra the dots having h=20 nm give contribution to the main peak centered at 1.72 eV, while dots having h=5 nm form high-energy tail centered at 1.79 eV. The difference between the emission energy of these dots (~70 meV) is reproduced well in calculations of optical transitions of the lens shape InP/GaInP QDs. The intermixing results in a higher band-gap of QD material, which is $Ga_{0.2}In_{0.8}P$, and shifts ensemble PL peak on ~60 meV. Negative degree of circular polarization was observed in the range 1.68-1.74 eV, which indicated electron accumulation of the dots having h=20 nm.

The spatially resolved near-field spectra we observed population of the dot by up to 20 electrons, as was reported by us previously [18]. This follows from the observation of a multi peak structure consisting of s-, p- and d-peaks and related to electron occupation of corresponding electronic shells, and a low energy tail of s-peak, which is shake-up (Stokes) component, related to the modes of relative and center-of-mass motion of electrons. The s-p splitting of the dots was 1-6 meV and it is approximately equal to the energy spacing of the levels of parabolic potential $\hbar w_0$. The some dots we see only Stokes component, which indicates that it contains a single electron. For these dots we observed a several <k|0>-transitions, *n*w0 which we assign to higher energy quantum confined levels.

The NF image of the emission intensity main peaks has lateral size at the base ~ 300 nm. We used these images to estimate the size of emission area of QD, which is ~50-150 nm and agree well with the calculations.

Wigner molecule versus charged exciton emission

We found that for single electron dots the number of shake-up <0|k>-transitions and distribution of their intensity dramatically depends on $\hbar w_0$: only two with <0|0> dominant were observed for $\hbar w_0$=4 meV and up to six with <0|2> dominant were observed for $\hbar w_0$=1.2 meV. The relative intensity of the transition are described very well by F_k of vibronic model giving *S* values 0.5, 1.5 and 2.5 and d_0=40, 110 and 140 nm for $\hbar w_0$=4, 1.8 and 1.2 meV, respectively. The d_0–values obtained corresponds to a dot size, which is unexpectedly, since calculations [19] give nearly two times smaller values.

We observed that in magnetic field a single elctron dot having $\hbar w$0=1.2 meV the energy of the s-peak increases with increasing of magnetic field, indicating that a stable 2e-WM is formed in photoexcited state of this dot.

For one dot we observed a single s-peak at zero field. For this dot s-peak shifts to lower energy up to 8T and at higher fields it starts shifted to higher energy. For this dot a Stokes component having energy 1.3 meV appears at 4 T and p-shell component having energy 2meV appears at 10 T. The measured low energy shift for B< 8 T is well reproduced by FD shift of doubly charged exciton (tetron). For higher field appearance of Stokes component and p-peaks indicated formation of Wigner molecule.

We also observed a mixed trion-WM behavior in which dot has two emission peaks one has negative, trion shif in magnetic field and the other positive, WM shiftt.

Conclusion

We study the emission spectra of single self-organized InP/GaInP QDs (size 100-220 nm) using high-spatial-resolution low-temperature (5K) near-field scanning optical microscope (NSOM) operating at magnetic field strength B=0-10T. The dots contain up to twenty electrons and represent natural Wigner molecules (WM). We observed vibronic-type shake-up structure in single electron QDs describing well by vibronic Frank-Condon factors and manifesting formation of two electron (2e) WM in photo-excited state. We used measurements of magnetic field shifts to distinguish emission of 2e-WM from singly charged exciton (trion). We also observed magnetic-field-induced molecular-droplet transition for two electron dot, having doubly charge exiton (tetron) in photoexcited state at zero field.

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TAIGA: A Large Multi-Component Detector for Gamma- and Cosmic Rays from a Few TeV to EeV Energy Regime

SCIENTIFIC ORGANIZATION

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ABSTRACT

TAIGA (Tunka Advanced Instrument for cosmic ray physics and Gamma Astronomy) is a large multi-component detector for studying celestial gamma ray sources and cosmic rays in the energy range from 10 to 12 degrees eV till ~10 to 18 degrees eV. One of the goal of TAIGA is to address such key problem in both high-energy gamma-ray astronomy and in cosmic ray physics as to find the galactic sources where the elementary particles are accelerated till PeV energies. In our presentation we are going to report on the status of TAIGA and about the first hints of a gamma-signal from a PeVatron candidate.

KEYWORDS

cosmic ray; gamma-ray astronomy; PeVatron; elementary particles; high-energy physics; Cherenkov light; EAS.

SUMMARY

TAIGA (**T**unka **A**dvanced **I**nstrument for cosmic ray physics and **G**amma **A**stronomy) is a large multi-component detector for studying celestial gamma ray sources and cosmic rays in the energy range from a few times 10^{12} eV till ~10^{18} eV. It is spread over an area of ~3 km^2 in Tunka Valley close to the Lake Baikal in Siberia.

TAIGA includes several types of detectors for identifying isotropic cosmic rays with high confidence level and for correspondingly efficient selection of several orders of magnitude less intense gamma rays from celestial sources. Cosmic gamma-rays and hadrons bombard the air molecules and atoms in earth's atmosphere and via chain of electromagnetic and nuclear reactions produce cascades of superluminal secondary particles. These emit Cherenkov light which is measured by the several detector components of TAIGA. While the operation principle of wide angle Cherenkov light integrating detectors of Tunka-133 (185 detector stations spread over ~3 km^2) and HiSCORE (currently 30 detector stations cover an area of ~0.3 km^2) is based on nanosecond fast-sampling of the light front by the largely spaced detector stations, the first Imaging Air Cherenkov Telescope (IACT) produces images of air showers. The surface and deployed in 2 m depth underground scintillation detectors of Tunka-Grande measure the number of muons, electrons and positrons. The radio emission from air showers is measured by Tunka-Rex (currently 46 stations).

The goal of TAIGA is to address several key problems in both high-energy gamma-ray astronomy and in cosmic ray physics. One of the most important problems of contemporary astrophysics and cosmic ray physics is to find the galactic

sources where the elementary particles are accelerated till PeV energies, i.e. to find PeVatrons, emitting gamma-rays at the energy range of ~100 TeV. The really innovative feature of TAIGA, dedicated to the search for PeVatrons, is the planned coincident operation of the IACT(s) and HiSCORE. This combination shall allow us to arrive at a huge collection area of the order of several km^2 at a very low cost. We plan to operate a single IACT with HiSCORE stations up to the shower impact distance of 600m. Currently it is not yet known how the IACTs operate in coincidence when their inter-telescope distance is well beyond 120m. There exist several Monte Carlo studies which, despite their non-completeness, predict that the telescopes could operate reasonably well till the inter-telescope distance of ~300m. At big heights the $e^{\pm}$ are still energetic and the Cherenkov light emission angle is larger or comparable to the multiple scattering angle. Most of this light will be impinging within a radius of < 150m from the shower core. When impact of a shower axis is beyond ~150m, most of the light is coming due to the multiple scattering of relatively low energy $e^{\pm}$ from low heights in a shower. Moreover, the measured light intensity is rapidly decreasing, so at a distance of ~300m there is about one order of magnitude less light than within ~150m.

Thus when the shower axis moves away from the telescope, the observed image has less and less photons and on top of that, it becomes progressively more truncated in height (i.e. the image parameter “length” becomes shorter and more “fuzzy”). This impacts the gamma-hadron separation power of the telescope.

For large impact distances 300-600m we plan to recover this loss of discrimination power of the IACT by using the shower axis impact point and direction information measured by the HiSCORE detector.

The second telescope of TAIGA will be set at ~300m away from the first one. It will allow us to scan the impact parameter range, at least along the connection line of the telescopes, up to which distance the telescopes can collect showers and reliably analyze them.

Thus the simple cell of the discussed instrument can be seen as a single IACT telescope surrounded by a number of HiSCORE stations, especially at the large impact distances beyond 300m. Because of the low-cost and simplicity of the HiSCORE station, such an array has a promise of being a very cost-effective one.

We want to prove that with the 600m operational range of a single IACT surrounded by HiSCORE, we can arrive at a detector, providing a collection area in excess of ~1 km^2 at high energies. Five such cells, for example, can cover an area in excess of 5.5 km^2, which is a very reasonable size for measuring PeVatrons at ~100 TeV energies in a reasonably short time.

Note that our approach is in strong contrast with the currently planned or being under design experiments like, for example, the Cherenkov Telescope Array (CTA), where 50-70 Small Size (~4m in diameter) IACT Telescopes (SST) are planned to be built in Chile for measuring the PeVatrons and the estimated cost of this array is ~45-50.-MEUR.

The total cost of TAIGA, assuming a similar performance as the CTA SST array, will be at least one order of magnitude less.

In our presentation we are going to report on the status of TAIGA and about the first hints of a gamma-signal from a PeVatron candidate.

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Spinodal decomposition in the Fe-Cr-Co ternary system

SCIENTIFIC ORGANIZATION

Materials Modeling and Development Laborotory (NUST «MISIS»)

ABSTRACT

Using the exact muffin-tin orbitals (EMTO) method based on the density functional theory (DFT) we have studied the tendency toward the spinodal decomposition of bcc Fe-Cr-Co solid solution. The ferromagnetic and the paramagnetic states were considered. Calculations of the lattice parameters, mixing enthalpy and Curie temperature were performed for both magnetic states. The calculations predicted that in the ferromagnetic state an increase Co and Cr content increases the tendency of Fe-Cr-Co alloys to spinodal decomposition, while in the paramagnetic state the alloys are stable.

KEYWORDS

Density functional theory, first-principles calculations, Fe-Cr-Co system, phase stability, spinodal decompositon, mixing energy.

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We would like to thank the Russian Foundation for Basic Reaserch (Grant № 14.Y26.31.0005) for financial support.

SUMMARY

Fe-Cr-Co hard magnetic materials have a unique combination of high magnetic properties with a corrosion stability, ductility and toughness. High mechanic properties make it possible to subject these alloys to cool and hot mechanic treatment and produce magnets with a different shape and size.

Hard magnetic properties in Fe-Cr-Co alloys can be reached by the formation of modulated structure during the spinodal decomposition into two isostructural phases: a (Fe-Co)-rich ferromagnetic phase (a_1) and a Cr-rich paramagnetic phase (a_2). A combination of thermomagnetic treatment and step-aging allows to reach a high-coercive state in these alloys [1]. Duration of these treatments strongly depends on alloys chemical compositions. For instance, in binary Fe-Cr alloys the high-coercive state have not been achieved as a result of slow atomic diffusion due to low decomposition temperature (710…790K) [2]. Thermal treatment methods are very sensitive to Co and Cr concentration, and depending on the concentration of alloys thermal treatment might last from 10 [1] to 100 [3] hours. In this respect, a knowledge of fundamental thermodynamic properties of Fe-Cr-Co system is highly desirable for the design of new magnetic alloys.

Unfortunately, there is quite limited experimental information about the thermodynamic properties of Fe-Cr-Co alloys. At the same time, the first-principles simulations allow one to obtain reliable description of the mixing thermodynamics of alloys with substitutional disorder, including magnetic alloys.

We have performed first-principles electronic structure and total energy calculations in the framework of the density functional theory (DFT) using the exact muffin-tin orbitals (EMTO) method combined with the coherent potential approximation (CPA) [4]. The disordered local moment (DLM) approximation was used for the description of the paramagnetic alloys [5]. In order to consider the effect of increasing temperature we have used the mean-field approximation in the configurational entropy calculations.

According to the calculations of Curie temperature the addition of Co (Cr) in Fe-Cr system the tendency to increase (decrease) in Curie temperature is observed, which does not contradict to the experimental data.

Starting by the results of the mixing energy calculations, in the ferromagnetic state $Fe_xCr_yCo_z$ solid solution decomposes spinodaly into two phases: (Fe-Co)-rich α_1-phase and Cr-rich α_2-phase, which is in a good agreement with experiment [1]. The local tendency to decomposition increases with the increasing of Co and Cr concentration.

So we can conclude that the theoretical modeling makes it possible to predict the most favorable decomposition directions and the chemical compound of the decomposition products.

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Advanced multi-photon imaging and diagnostics with quantum dot-based hybrid nanostructures

SCIENTIFIC ORGANIZATION

Université de Reims Champagne-Ardenne

ABSTRACT

An ideal multiphoton fluorescent nanoprobe should combine a nanocrystal with the largest two-photon absorption cross section and the smallest highly specific recognition molecules conjugated with a nanoparticle in an oriented manner. However, the conditions used for conjugation of conventional antibodies (Abs) often provoke their unfolding and yield nanoprobes with irregular orientation. Conjugation of Ab-fragments, such as single-domain antibodies with nanocrystals is an attractive approach to generation of ultrasmall and highly specific diagnostic nanoprobes.

KEYWORDS

Quantum dots; imaging; diagnostics; FRET

ACKNOWLEDGEMENTS

This work was supported by the Federal Target Program for Research and Development of the Ministry of Education and Science of the Russian Federation (grant no. 14.584.21.0012, contract no. RFMEFI58415X0012).

SUMMARY

Cancer remains one of the leading causes of death in the world. The use of a panel of proven biomarkers (instead of single biomarkers) can significantly improve the sensitivity and efficiency of diagnosis. Advanced multiplexed imaging with quantum dots (QDs) may become an indispensable tool for early cancer diagnostics[1].

An ideal single- or multiphoton fluorescent nanoprobe should combine a nanocrystal with the largest single-photon (1P) or two-photon (2P) absorption cross section (ACS) and the smallest highly specific recognition molecules conjugated with a nanoparticle in an oriented manner[2,3]. However, the conditions used for conjugation of typical recognition molecules (conventional antibodies, Abs) with nanoparticles often provoke their unfolding and yield nanoprobes with irregular orientation of Abs on the nanoparticle surface. Conjugation of smaller Ab fragments, such as single-domain antibodies (sdAbs), with QDs in an oriented manner can be considered as

an attractive approach to generation of ultrasmall diagnostic nanoprobes[2].

CdSe/ZnS QDs conjugated to 13-kDa sdAbs derived from camelid IgG or streptavidin have been used as efficient 1P- or 2P-excitation probes for imaging of carcinoembryonic antigen (CEA), HER2, and other biomarkers[2-4]. The 2P-ACS for some conjugates is higher than 49,000 GM (Goeppert-Mayer units), which is close to the theoretical value calculated for CdSe QDs (50,000 GM)[3] and considerably exceeds that of organic dyes.

High-quality imaging in medical practice requires clear discrimination between the fluorescence of immunostaining probes and the autofluorescence of biological liquids and tissues. 2P-microscopy with excitation in the near-IR spectral region has now become the main fluorescence imaging technique for thick biological specimens, because the excitation band is far from the spectral region of tissue autofluorescence excitation and enables deep imaging of biological tissues.

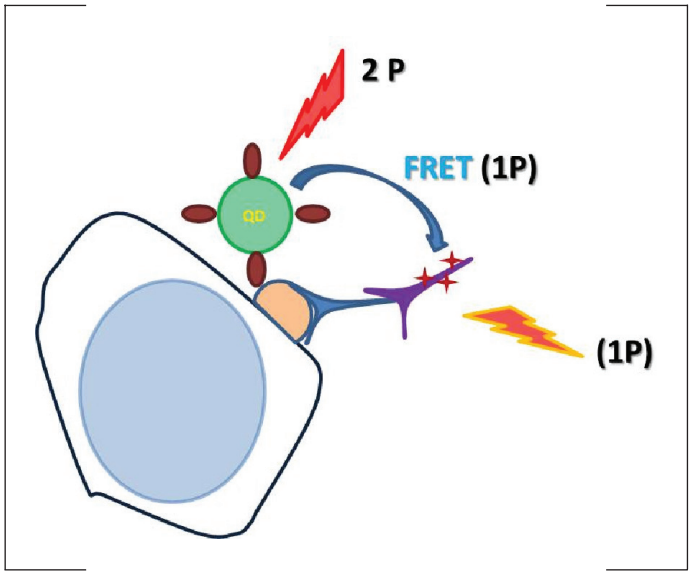

Figure 1. Two-photon (2P) excitation of the immunostaining complexes for MC38 cells overexpressing carcinoembryonic antigen (CEA).

The sample is labeled with oriented conjugates of quantum dots and single-domain antibodies (sdAbs) and, additionally, with a primary antibody labeled with the AlexaFluor dye forming an efficient donor/acceptor pair with the QD.

A further step in this direction has been made in our study (Figure 1). Here, efficient FRET under 2P excitation was demonstrated for the double immunostaining complexes formed on the surface of MC38 cancer cells overexpressing CEA with the use of sdAb-QD conjugates (donor) and a combination of the monoclonal Ab against CEA and the secondary antibody labeled with the AlexaFluor dye (acceptor).

The proposed approach permits obtaining an exceptional contrast of 2P imaging of cancer biomarkers without any contribution of cell and tissue autofluorescence in the recorded images thus paving a way to advanced diagnostics with the use of highly oriented conjugates of sdAbs with the colloidal nanomaterials.

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Experience of designing application readout ASIC in the ASIC Lab of NRNU MEPhI

SCIENTIFIC ORGANIZATION

National Research Nuclear University MEPhI

ABSTRACT

The laboratory of ASIC design was created in NRNU MEPhI to develop the design of a specialized microelectronic component base in Russia. An important direction of the laboratory works is the creation of ASIC for reading out the signals of the CBM experiments muon chambers. This chip processes the gas detector signals determining this amplitude, time stamp and the number of channel in which the signal has been detected, and finally provides its output at a frequency of 320 MHz. The results of testing and measuring the prototypes of chip are presented.

KEYWORDS

Analogue electronic circuits; Front-end electronics for detector readout.

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation (grant №14.A12.31.0002) in accordance with the RF government order № 220.

SUMMARY

The Laboratory of ASIC design was created on the basis of NRNU MEPhI (ASIC Lab) under the contract No. 14.A12.31.0002 in the premises NRNU MEPhI total area of 110 m2. The Infrastructure of the ASIC LAB includes a seminar cluster, design lab, test laboratory (clean room).

The seminar cluster of the established laboratory is used to conduct workshops and design courses. Using the means of the seminar cluster, we held two All-Russian Conferences on the Design with the Cadence CAD [1] [2].

The design cluster is equipped with everything needed for design - these were acquired two powerful servers (16 cores at 3.2 GHz), and 15 client stations, the design is carried according to the client-server scheme. In the lab servers there have been installed advanced software of computer-aided design (CAD) of the US companies Cadence Design Systems and Mentor Graphics. The laboratory has licensing agreements with several leading companies (TSMC, GlobalFoundries, UMC, AMS, AMIS, Micron) to provide design kits for designing with design rules from 350 to 40 nm. The designed chips are manufactured via the European Europractice organization – NRNU MEPhI is leader by the number of manufacture runs among Russian companies (fig. 1) [3].

Figure 1 Number of manufacture runs among Russian companies.

Russia		
Budker Institute of Nuclear Physics	Novosibirsdk	4
IPMCE	Moscow	3
JSC "NTLAB"	Moscow	2
Moscow Engineering Physics Institute	Moscow	20
Moscow Institute of Electronic Technology	Moscow	5
Moscow Institute of Physics and Technology	Moscow	5
N.I. Lobachevsky State Univ	Nizhni Novgorod	8
SRIET-SMS CJSC	Voronezh	6
TUSUR university	Tomsk	2
University St Petersburg	St Petersburg	6
Vladimir State university	Vladimir	1

The fabricated chips are tested in the laboratory and measuring cluster ASIC LAB. For accurate measurements in NRNU MEPhI these was created a clean zone of the ISO class 7, and purchased the latest Agilent and National Instruments measuring equipment, as well as a Cascade probe station(fig.2) and antistatic furniture. The created cluster ensures accurate testing of analog-digital ASICs.

Figure 2 Measuring equipment and probe stationt

The main directions of the laboratory works are: equipment for large physics experiments, specialized electronics for the aerospace industry, the chips for solving some applied mathematics. The leading scientist of ASIC Lab Samsonov VM has extensive an experience in the development of equipment for the international experiments such as STAR, Fenix, Atlas, CBM.

One of the applications that the laboratory is working at, is the creation of multi-channel electronics for the gas (GEM) detectors of the muon chambers compressed baryonic matter (CBM) at the FAIR accelerators (Darmstadt, Germany) [4]. GEM detectors will be operating at a high gas gain in the range of 1000 to 8000. The MUCH set up has 25,000 64-channel chips to handle totally 1.5x106 channels. Also the GEM muon chambers will have projective segmentation with the smallest pad size being as small as 4.1 x 4.1 mm2 in the inner region and as large as 2.1 x 2.1 cm2 in the outer region of the chamber. This sets up the following ASIC features:

- Dynamic range of 1 - 100 fC;

- Wide Cdet range of 1 - 50 pF;

- S / N maximization at the periphery pads;

- Hit rate up to 1 MHz at the central pads;

- Low (less than 10 mW / channel) power consumption;

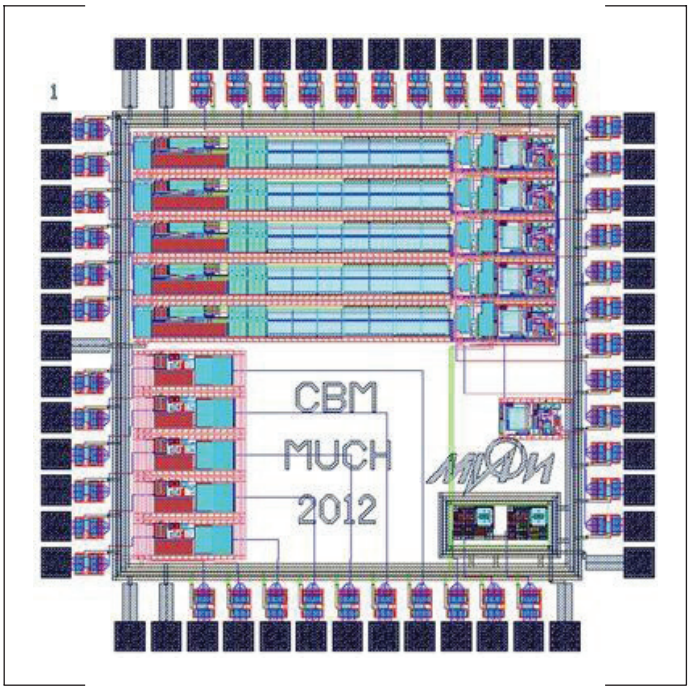
- Area efficiency for all building blocks and ADC as the most critical one.

The route design complexity analog-digital chips consist of several steps of chip prototyping. At the first stage the IP blocks of which the chip consists are designed. The next interaction watches the IP units with each other and composes them together, to form a system. If the results of laboratory testing of the system meet the specifications for the chip the design is performed and full-scale chip launched. Otherwise some additional launches of IP blocks and other elements of the system are carried out to ensure the operation of the system.

At the present moment there have been made 4 launches of the chip prototype of the ASIC, reading out the muon chamber signals.

The first prototype ASIC (fig. 3) contains two preamplifier versions [5]. One version includes a traditional structure of a charge-sensitive amplifier (CSA), followed by the shaper. In the other version of the preamplifier, the shaper functions are integrated into the CSA schematic. Due to passive elements, the area occupied on chip by the channel version containing the separate shaper is much larger than the alternative version (1050 × 100 um^2 versus 200 × 100 um^2). Both versions of processing channels ensure commensurable noise characteristics. In this case, the structure with a separate second order shaper allows us to reach the necessary noise characteristics at a lower power consumption than the version without shaper. At the same time, due to the large area occupied by the passive elements of the standalone filter (the versions differ in areas by a factor of 5), the version with the filter becomes less preferable for use in multichannel systems.

Figure 3 First prototype CBM MUCH



The second prototype (fig. 4) includes 8 analog processing chains, 2 threshold DACs, 8 SAR ADCs and a digital part) [6].

Each analog channel contains the preamplifier, followed by two shapers (fast and slow) and differential comparator. The preamplifier is based on the folded cascode CSA architecture with additional gain boosting. The preamplifier gain is set to 5 mV / fC and its noise level is estimated by ENC = 1000 el at 50 pF. Since CBM MUCH GEMs will have different granularity, the requirements to the front-end electronics are also

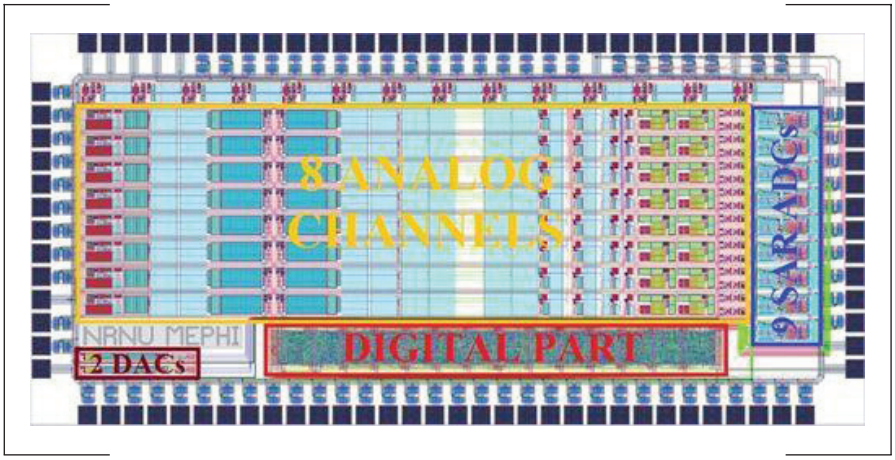
different for the central and peripheral parts. Thus, the preamplifier is followed by two chains: a slow channel optimized for S / N ratio in order to use it in the periphery, and a fast channel, adapted to the hit rate of the inner detector part, where the occupancy is the highest. Both channels are realized with CR-RC shapers with different peaking times, 60 ns and 260 ns accordingly.

The structure of the prototype includes a single-ended 40 MS / s 6-bit SAR ADC [7] with asynchronous architecture and an internal high speed 500MHz clock, generated by dynamic comparator, is used. Moreover, a fully dynamic comparator with near to zero static power consumption. That flip-flop type uses gate capacitance to store the input. Clocking at 500MHz allows to save up to 80% of power, comparing with a conventional D flip-flop, based on NAND gates.

The digital control and readout block plays the role of the backend part of ASIC. Backend collects data from the ADC and organizes their serial output from the chip. For the data exchange the non-standard protocol was implemented. Backend operating frequency is 320 MHz.

The main parameters of the first ASIC prototype are: dynamic range of 100 fC, ENC of 1000 e- at 50 pF, power budget of 10mW per channel. Its structure contains area efficient (0.0255mm^2) 1.2mW at 50 Msps 6-bit SAR ADC in each channel.

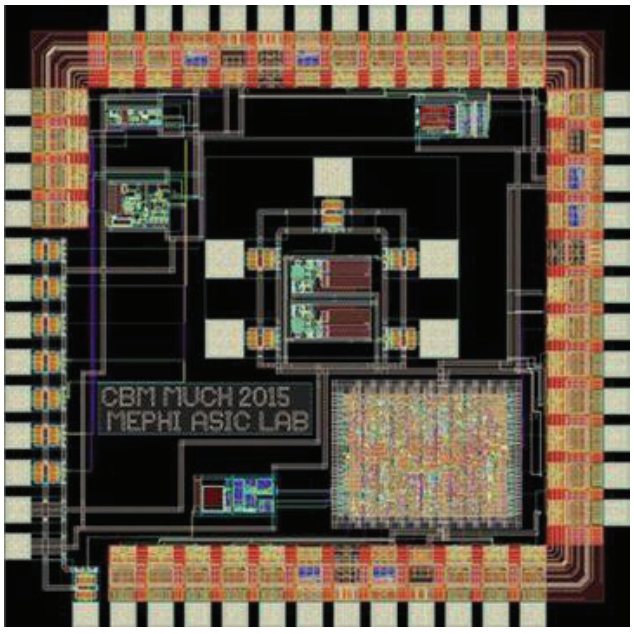
Figure 4 Second prototype CBM MUCH



Subsequent testing showed the prototype performance, however, revealed problems with the system elements in the crystal - error shred generation and ADC digital logic, poor accuracy of threshold DAC, self - excitation in the comparator block.

The test chip (fig. 5) (CBM TEST) includes the units of ADC-DAC, SLVS transmitter and receiver, the digital unit of information acquisition. The SLVS transmitter consumes 4.9 mW at 1.8 V supply voltage and provides transmission speed up to 320 Mbps and 2 mA output current. The SLVS receiver consumes 500 uW at a 1.8 V supply voltage and a 320 Mbps speed. The optimized DAC circuit is more resistant to the technological spread has improved parameters of integral nonlinearity, full scale error and a reduced power consumption. The basic DAC parameters are: LSB = 200 nA, power consumption of 25 mW, the bit numbers of 5 occupied area- 206 x 100 um. The errors in the ADC circuit have been corrected namely the errors in the performance of comparator and digital logic. The main parameters of the ADC are: bit numbers - 6, LSB- 28 mV, effective number of bits - 5.86, SINAD- 37 dB, SNR- 37 dB SFDR -43,3 dB, power consumption 2 mW, signal frequency - 500 kHz, sampling frequency - 40 MS / s, occupied area - 176 x 90 um^2.

Figure 5 ASIC with test blocks (CBM TEST)



The design of the digital data acquisition and output unit – has been completed signals are receiving a frequency of 40 MHz and put out at a frequency of 320 MHz, the unit's power consumption - 10 mW occupied area - 460 x 360 um.

Using the experience of designing the second prototype of the CBM TEST ASIC, there was developed the third chip (fig. 6) [8] prototype for the detectors of the CBM MUCH muon chambers.

The structure of the prototype includes: 2 full readout channels, 2 SAR ADCs, Digital control, DACs, Timestamp, Digital peak detector, SLVS Transmitter & Receiver, ELT test blocks. Blocks of readout channels, ADC, DAC, SLVS Transmitter & Receiver were taken from the second prototype ASIC and CBM TEST. Significant changes have been made in digital logic unit (Backend) which includes Digital control units, Digital peak detector, Timestamp. The Backend performs

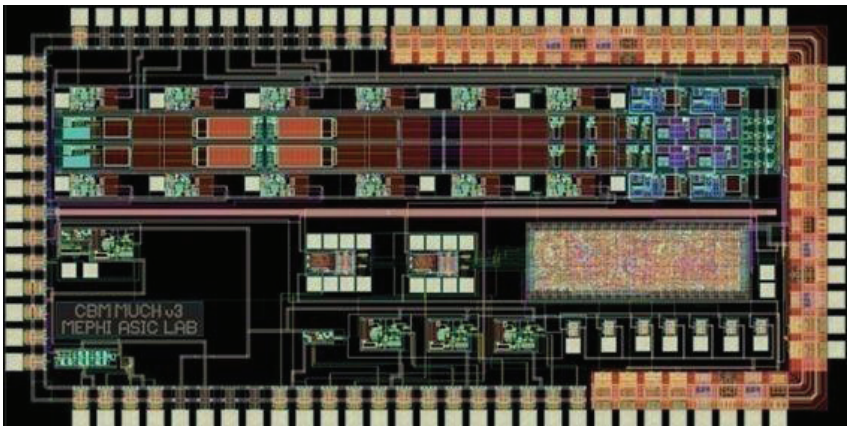


Figure 6 Third prototype CBM MUCH

Figure 7 Prototype of detectors and test board

the following functions - provides operations of data exchange and output of results, control operations of ADC and DAC performance, clock generation, time stamp fixation, the formation of the code of the input signal peak value.

Prototypes of the detectors have been studied with the prototype front-end ASIC (fig. 7, 8). A prototype (fig. 9) read-out system is being developed jointly by PNPI and NRNU MEPhI. The system prototype includes the gas-filled detector based on the GEM and TGEM technologies, gas and high voltage (HV) system and the front-end electronic prototype. To get the stable GEM diode voltages, active dividers are used in the HV system. The front-end prototype consists of the test PCB with the read-out ASIC with the external transient voltage suppressors (TVS). TVS were used to prevent the input ASIC breakdowns due to the GEM detectors sparks. The Test PCB includes the input/output analog and digital interface for data exchange with FPGA processing board. The low-power voltage distribution system on PCB utilizes the FEASTMP DCDC converter. As a multichannel analyzer the CAEN DT5742 digitizer was used. The measurements were carried out with the Ar/CO_2 gas mixture and the ^{55}Fe source. ^{55}Fe spectrum were obtained. The measured noise of 1000 electrons at 20pF input capacitance increases up to 2500 electrons at input capacitance of 80 pF.

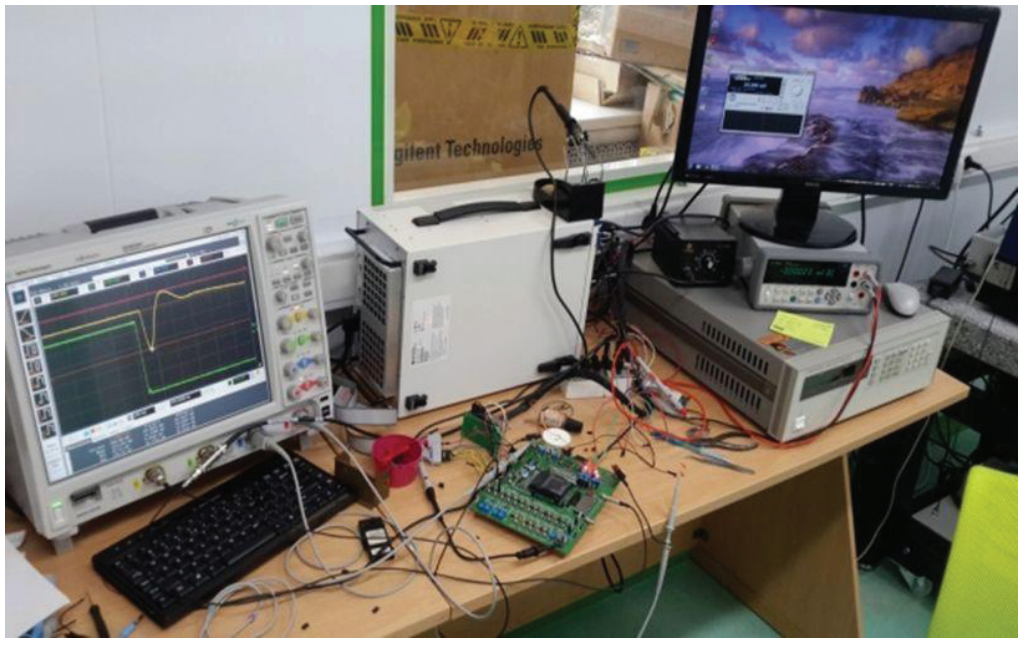


Figure 8 Measured ASIC with equipment

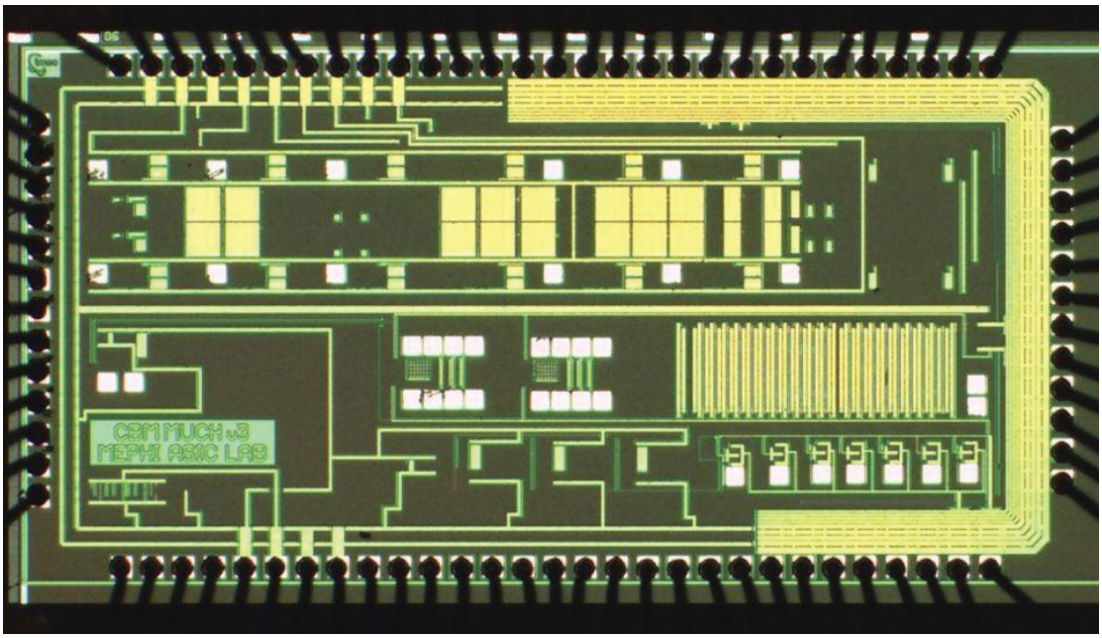


Figure 9 Manufactured third prototype

Analyzing the results of studding third prototype, there is designed of 32-channel chip, which includes the following options - full-size BackEnd, 8-bit SAR ADC, an improved peak detector, I2C and the Protocol MUCH ASIC – GBTx. The works on designing the chip for reading out the signals from the detectors of the muon chambers are carried out in accordance with the plan described in the TDR[9].

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Laser writing with sub-nanosecond burst of femtosecond pulses

SCIENTIFIC ORGANIZATION

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ABSTRACT

A method of efficient laser micromachining in bulk of fused silica and sapphire with a burst of femtosecond pulses separated by 10 – 100 ps is proposed and demonstrated. We used Fabry-Perot cavity to split the NIR 180 fs pulse into a burst with the same duration of each pulse in the burst. The new method exploits strongly localized absorption by transient electronic excitations prepared by the first pulse in the burst. In comparison with a single pulse an increased refractive index change and birefringence is obtained by a single burst.

KEYWORDS

Laser direct writing, refractive index change, birefringence, burst of femtosecond pulses.

ACKNOWLEDGEMENTS

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SUMMARY

1 Introduction

Femtosecond laser direct writing and micromachining attract considerable interest for a variety of applications ranging from integrated optics and microfluidics to printable flat optics and multi-dimensional optical data storage. Micromachining with temporally shaped pulses or femtosecond pulse trains that exploit material dependent relaxation processes has been applied for creating sub-wavelength features via control of ionization processes on a sub-picosecond time scale [1], and writing waveguides with a circular cross-section via control of a heat deposition with sub-microsecond bursts of femtosecond pulses [2]. There is lack of experiment sub-nanosecond burst. Nevertheless an enhancement of strength of the nanograting form birefringence was observed under writing with train of pairs of pulses, when interval between pulses was less then nearly 50 ps presumably due to increased absorption of self-trapped excitons (STE) [3]. Results of this work allowed us to suggest that one or few bursts of pulses, separated by few decades of picosecond would efficiently produce material modification, and this efficiency would go down with pulse separation increase according to STE decay. In our experiments we have generated such bursts, and found that it is a really efficient tool for refractive index modification and forming of a birefringence structure. However we observed an unexpected dependency of the refractive index change upon pulse separation interval, which is inconsistent with simple decay of STE.

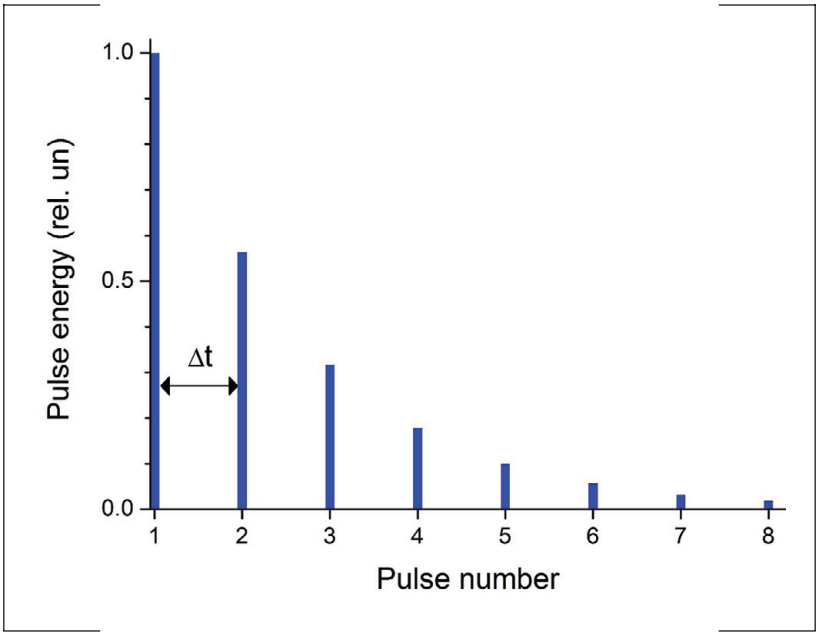

Fig.1 Schematics trace of a burst of femtosecond pulses, generated by Fabry-Perot cavity with the 75 % reflection coefficient of each mirror.

2 Writing with sub-nanosecond burst

IR laser femtosecond modification creating permanent refractive index change is initiated by multiphoton ionization, which is followed by linear absorption by the electron plasma, multiphoton absorption of self-trapped excitons (STE) and avalanche ionization [4]. In the experimental setup we used Fabry-Perot cavity to split the 180 fs pulse at 1030 nm into a burst of pulses (Fig.1). Pulse separation in the burst Δt was equaled to 10 -70 ps defined by

the cavity length. The first pulse with the highest energy was followed by train of pulses with exponentially decreasing pulse energy. Effective burst duration could be achieved about 10 times greater compared to the duration of tailored pulse produced by the third-order chirp without stretching of each pulse in the burst [1]. Such temporal form of the burst allowed localizing modification in the beam waist due to reduction the energy of the first pulse down to the inscription threshold energy, and at the same time strong modification is produced due to absorption of the subsequent pulses by electron-hole plasma or STE [3-5].

Absorption of the subsequent pulses is more efficient, than the first pulse absorption, because the lower number of photons is required for an absorption act for subsequent pulses by transient electronic excitation. On the other hand this absorption is localized in the region prepared by the first pulse, thus strong localized modification with refractive index change is produced.

3 Charaterization of modifications and discussions

We found, that burst of pulses produce modification of refractive index with higher phase delay than one pulse by factor of 2 - 5, and the phase delay monotonically increases with increase of pulse separation interval Δt (Fig.2) in the range of 0-20 ps and then the dependence is saturated. In fused silica the single pulse modification with pulse energy just above inscription threshold causes the positive refractive index change, and pulses with higher energies produce negative changes of index, while bursts of pulses always produce modification with negative refractive index change for burst energies above the inscription threshold energy as in fused silica, so in sapphire doped with Ti^{3+}.

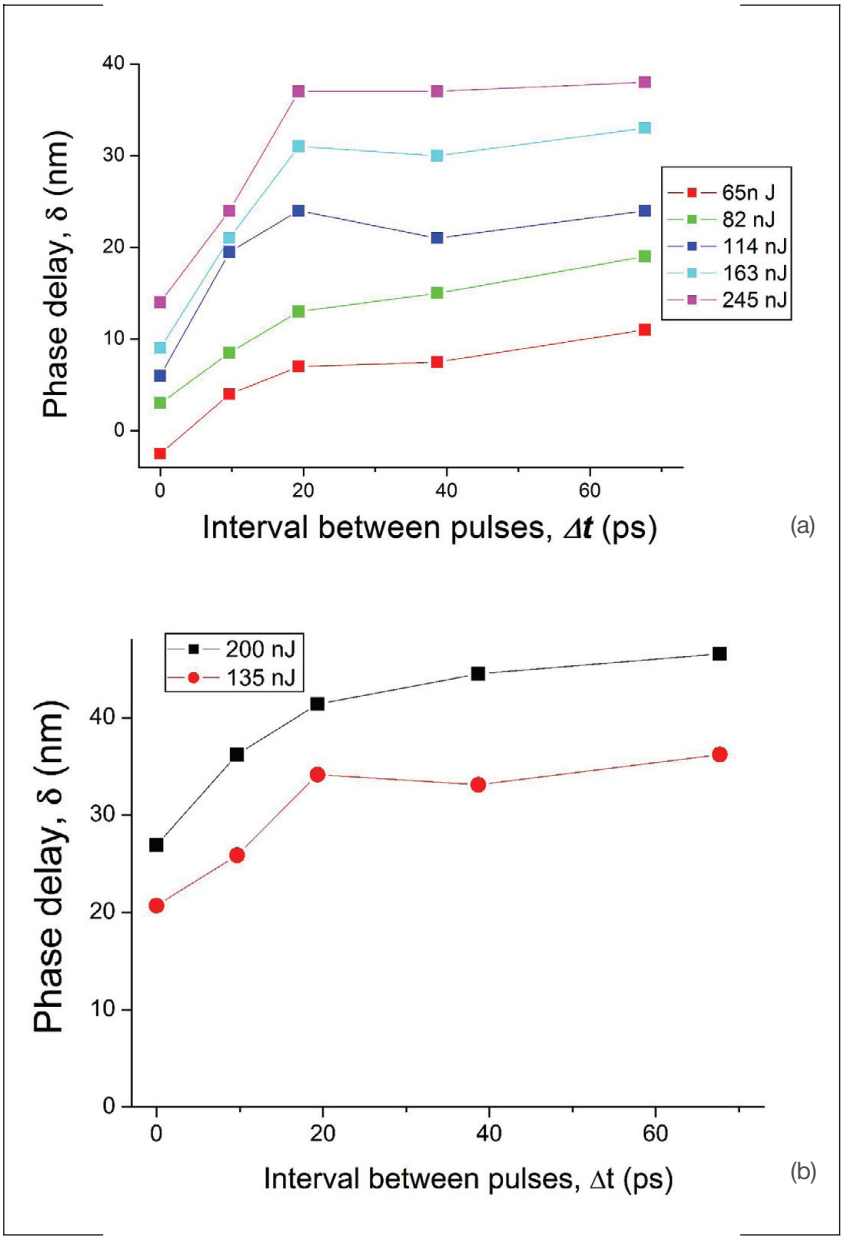

Fig. 2. Phase delay due to the single burst modification of refractive index in fused silica (a) and in sapphire doped with Ti^{3+} (b) in dependency on the pulse separation interval. Zero interval corresponds to a single pulse. Positive phase delay corresponds to negative refractive index change in our notations. Labels on the graph denotes burst energy. Focusing lens - NA=0.65.

Phase delay increase on the scale of 0 - 20 ps is inconsistent with known electronic relaxation processes, in particular, with dynamics of formation and decay of STE in SiO_2, and electron-hole plazma and self-shrunk excitons (SSE) in Al_2O_3 [6]. We suggest that the observed increase reflects intrinsic dynamics of excitation relaxation inside STE and SSE. Probably there are two channel for localized excitons transformation in presence of intense laser pulse: 1) back excitation to electron-hole plazma; 2) decay to stable structure defects causing refractive index change, and we suggest that after last transformation the probability of recurrent excitation to electro-hole pair dramatically drops down. It was shown that in fused silica under high density of excitation accompanying STE Frenkel defects are further transformed into stable defects [7]. Taking into account that only the second channel of STE and SSE transformation exists between pulses in the burst, one can conclude that, density of the stable defects increases with enhancement of pulse separation interval. In Al_2O_3 the phase delay dependence is less pronounced, than in SiO_2. This is obviously connected with lower role of SSE in defect formation, as lifetime of free electron in this crystal is about 100 ps. In sapphire the subsequent pulses in the burst must be absorbed by electron-hole plazma too, and holes could be localized on Ti^{3+} ions with creation of stable Ti^{4+} ions.

Increased efficiency of burst absorption is confirmed in measurements of one pulse/burst transmittance T in dependency on pulse /burst energy under the same focusing conditions

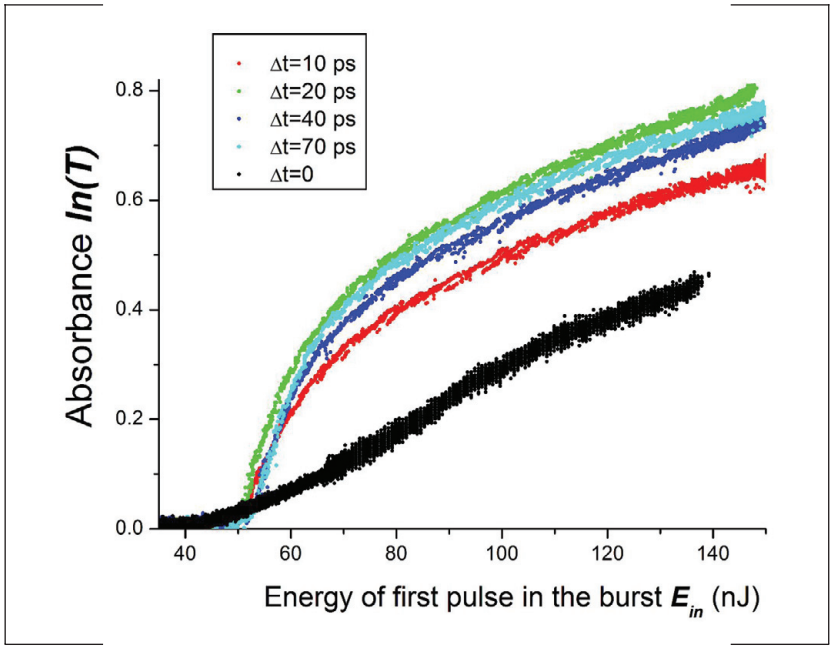

Fig. 3. Absorbance *ln(T)* of a pulse (black points) and a burst (red points) in fused silica in dependency on the pulse energy or a first pulse in the burst energy. Intervals between pulses equal to 10 ps (red points), 20 green points, 40 ps (cyan points) and 70 ps (blue points). Focusing lens - NA=0.65.

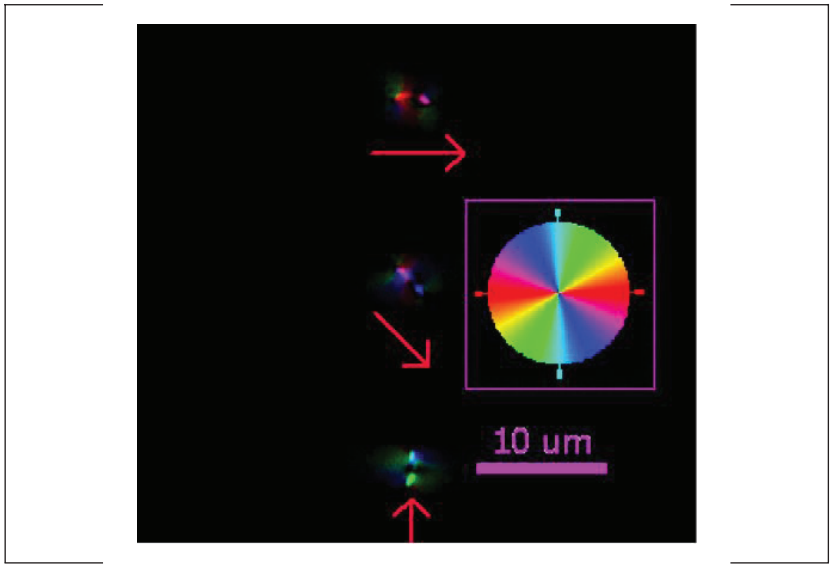

Fig. 4. Microscopic pictures of birefringent spots, produced by the burst of femtosecond pulses. Colors code direction of slow axis in accordance with the legend. Red arrows show direction of laser beam polarization. Burst energy is equaled to 110 nJ. Focusing lens - NA=0.65.

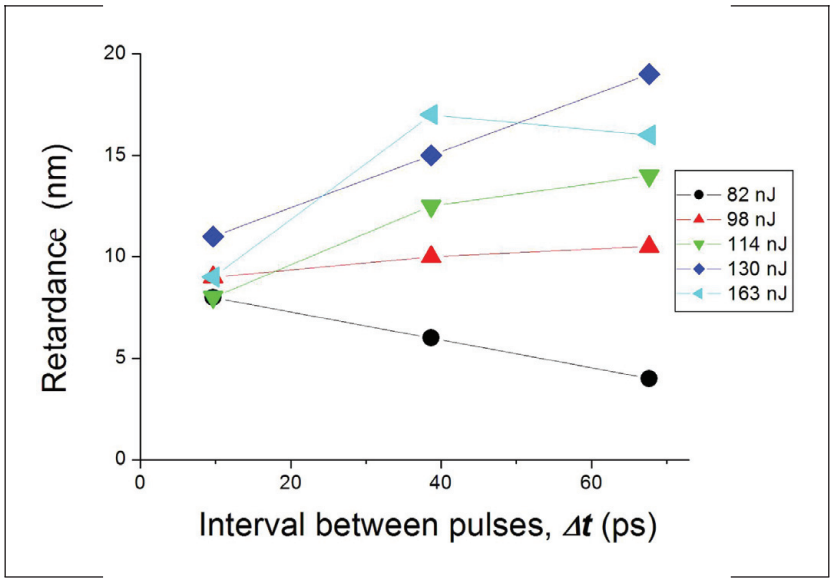

Fig. 5. Retardance under single burst modification in fused silica in dependency on the pulse separation interval.

in fused silica (Fig.3). Energy meter head was placed closely behind the thin glass plate so that 100% of laser radiation focused in the plate at the 100 μm depth by a lens with NA=0.65, went through the plate and then collected by the head. The glass plate was placed on a high precision translation stage, which was moving perpendicular to the focused laser beam, thus each laser shot produced an excitation in a new glass area. Transmittance curve of a single pulse has a recognizable shape [3], while dependence of absorbance for the burst is dramatically differed with a sharp increase at the energy close to modification threshold and higher absorption at higher energies.

It was found, that in contrary to a single pulse, absorption of the burst with the same total energy is strong enough to produce a birefringent micro-structure in fused silica. It consists of two elongated birefringent spots with parallel slow axes separated by area without birefringence (Fig.4). The slow axis of birefringence and direction of elongation of inscribed pattern follow polarization of the femtosecond beam.

Dependence of birefringence retardance upon the interval between pulses in the burst is not so definite as for phase delay, and its slope depends on the burst energy (Fig.5). There is small difference in retardance for different energies at the 10 ps interval, and diversity arises when the interval increases. There is no detectable birefringence for a single pulse.

Conclusion

In conclusion we have proposed and demonstrated a method of efficient micromachining with the burst of laser pulses separated by time interval 10 - 100 ps. Such burst produces enhanced refractive index change and a birefringent structure even with one laser shot due to increased pulse absorption. Nature of unexpacted dependence of refractive index change upon pulse separation interval in the burst could be connected with relaxation processes in localized excitons.

This work was supported by Advanced Research Foundation and Ministry of Education of Science of Russian Federation, grant #14.Z50.31.00J. Hernandez-Rueda, N. Gotte, J. Siegel, M. Soccio, B. Zielinski, C. Sarpe, M. Wollenhaupt, T. A. Ezquerra, T. Baumert, and J. Solis, “ACS Appl. Mater. Interfaces **7**, 6613–6619 (2015).

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ADDITIONAL INFORMATION

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Transmission and Reflection Spectra of Photonic Crystal with Plasmonic Defect Layer

SCIENTIFIC ORGANIZATION

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ABSTRACT

Polarization-dependent features appearing when the electromagnetic wave is reflected from and transmitted through a 1D photonic crystal with a defect layer formed by nonspherical metal nanoparticles are theoretically studied.

KEYWORDS

Photonic crystals ; Nanomaterials ; Polarization - selective devices.

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation (Project No.14.Z50.31.0015).

SUMMARY

When used as inclusions in dielectric matrix, metal nanoparticles allow obtaining composite materials with optical properties vastly different from that usually found in natural materials. Absorptive and dispersion properties of such media are determined by the frequencies of the plasmon resonances, which depend on the shape of impurity metallic nanoparticles. Therefore the composite material with uniformly oriented elongated nanoparticles behaves like a dichroic crystal. Vetrov et al. investigated the relationship between the structural parameters of a plasmonic nanocomposite and the spectral properties of the photonic crystal structures. In this work the possibility of using plasmonic nanocomposite with nonspherical inclusions as a tuning defect in a photonic crystal (PC) is considered and the features of the behavior of electromagnetic eigenmodes in an artificial layered periodic structure with a finite number of periods a nd a plasmonic defect are analyzed.

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Wide-angle atmospheric Cherenkov array TAIGA-HiSCORE

SCIENTIFIC ORGANIZATION

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ABSTRACT

TAIGA-HISCORE, deployed in the Tunka Valley (50 km west of Lake Baikal), is one part of the planned integrated gamma observatory TAIGA intended for investigations in the field of high-energy (>30 TeV) gamma-ray astronomy and cosmic-ray physics as well as the search for dark matter. The brief array description, estimation of energy threshold, measurement of angular sensitivity and time-calibration as well as first results from operating a prototype array composed of nine stations spread over an area of ~0.1 square kilometers during the winter of 2013–2014 are presented.

KEYWORDS

Cosmic ray; gamma-ray astronomy; PeVatron; elementary particles; high-energy physics; Cherenkov light; EAS.

SUMMARY

TAIGA-HISCORE is wide-angle non-imaging atmospheric Cherenkov array. Its appellation is abbreviation, deciphered as the **T**unka **A**dvanced **I**nstrument for **G**amma-ray and cosmic ray **A**strophysics - **H**igh **S**ensitive **C**osmic **OR**igin **E**xplorer.

The array consists of optical stations, located at the lattice point. The distance between the closest neighboring stations is around 106 m. There are 28 OS in area of 0,25 km2 at this stage of deployment (2016).

Each optical station consists of four optical modules – photoelectric multipliers with photocathodes 20 cm in diameter, equipped by Winston cones, which fourfold enlarge the light collecting area of each photomultiplier. The station's solid angle of view is 0,6 sr. To lower the station's energy threshold, the signals from the anodes of the four photomultipliers are added together, and the total signal is fed to the comparator input of the local triggering system. The signals from the photomultiplier anodes and intermediate dynodes are digitized at a sampling rate of 0.5 ns. The comparator threshold of the local triggering system is selected to lie in the region where the amplitude spectrum of the signals generated by an EAS (density spectrum) intersect with the fluctuation spectrum of the night sky background. The station's count rate is 12–16 Hz. The modeling of the count rate of a single station showed that this count rate corresponds to a threshold Cherenkov light flux of 0.3 photons per square centimeter. With this threshold, an EAS generated by 30 TeV gamma quanta should be detected at distances of up to 120 m from the shower axis and an EAS generated by 30 TeV protons should be detected at distances of up to 50 m from the shower axis.

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Flux-flow oscillators based on high temperature superconductors

SCIENTIFIC ORGANIZATION

Institute for Physics of Microstructures of RAS

ABSTRACT

The results of current development in IPM RAS of fabrication technologies of Josephson junctions based on high-temperature superconductors are presented. We describe the peculiarities of new magnetron sputtering technique of YBCO thin films on YSZ bicrystal substrates and show current-voltage characteristics of the junctions, demonstrating visible flux-flow steps. Besides, we describe the development of original wet etching technology for fabrication of BSCCO standalone mesas.

KEYWORDS

Flux-flow oscillators, high temperature superconductors, YBCO, BSCCO.

ACKNOWLEDGEMENTS

The work is supported by Russian Science Foundation grant N 16-19-10478.

SUMMARY

The results of current development in IPM RAS of fabrication technologies of Josephson junctions based on high-temperature superconductors are presented. We describe the peculiarities of new magnetron sputtering technique of YBCO thin films on YSZ bicrystal substrates and show current-voltage characteristics of the long Josephson junctions, demonstrating visible flux-flow steps. For the opposite magnetic field directions, the flux-flow steps with significantly different height and slope are observed [1]. It is demonstrated that the most probable reason of this discrepancy is recently predicted asymmetry of spatial bias current distribution due to crystallographic anisotropy of bicrystal substrates [2]. We have also studied the Shapiro steps of the fabricated structures. The fractional Shapiro steps with various numbers of visible substeps depending on junction lengths are observed both experimentally and theoretically. Besides, we describe the development of original wet etching technology for fabrication of BSCCO standalone mesas [3]. The produced mesas can be made much thicker than ones usually being studied (roughly from 1 to 20 um). The time required for the fabrication is much smaller in comparison with the standard method of ion milling. The process used is controllable which provides acceptable precision of mesa fabrication. The IV characteristics of the sample showing Josephson nature were obtained.

The work is supported by Russian Science Foundation grant N 16-19-10478.

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ADDITIONAL INFORMATION

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Diamond refractive lenses for diffraction-limited x-ray sources

SCIENTIFIC ORGANIZATION

Immanuel Kant Baltic Federal University

ABSTRACT

In view of the global switch to the diffraction-limited fourth generation X-ray sources, there is a growing need for X-ray optical elements fabricated from materials that can withstand extreme heat and radiation loads. Diamond can satisfy all the requirements and in our research, for the first time single-crystal diamond planar and 2D refractive lenses were fabricated by laser micromachining in up to 1.2 mm thick diamond plates. Various lenses with apertures up to 1mm and radii of the parabola apex up to 500μm were tested in the focusing and imaging modes.

KEYWORDS

X-ray optics, X-ray refractive lenses, diamond machining, X-ray sources.

ACKNOWLEDGEMENTS

Work was supported by the Ministry of Education and Science of the Russian Federation: Grant Nos. 14.Y26.31.0002 and 02.G25.31.0086.

SUMMARY

The intensive development of X-ray refractive optics' instrumentation and tools has given birth to X-ray refractive lenses [1] which are now the standard elements at third-generation synchrotron radiation sources. In view of the global switch to the fourth generation of synchrotron sources and X-ray Free Electron Lasers, there is a growing need for x-ray optical elements fabricated from materials that can withstand extreme heat and radiation loads while still providing effective focusing and imaging. Diamond can satisfy all the requirements provided that a suitable lens manufacturing technology is available.

In our research [2], for the first time diamond planar refractive lenses were fabricated by laser micromachining in up to 1.2 mm thick diamond plates (both mono- and polycrystalline) which were grown by CVD and HPHT. Various linear lenses with apertures up to 1mm (fig.1) and radii of the parabola apex up to 500 μm were manufactured and analyzed with SEM, AFM, Raman spectroscopy and, of course, X-ray tests at the European Synchrotron Radiation Facility (ID06 beamline). A uniform intensity of the image of the focused X-ray beam showed the high quality of the lens's side walls and profile allowing to focus the X-radiation in accordance with the lens' demagnification factor. Planar lenses were followed by 2D parabolic X-ray refractive half lenses (fig. 2), which were also manufactured by laser micromachining of single-crystal diamond. A single 2D lens had an aperture of 1 mm and parabola apex radii of 200 μm. Forming a compound refractive lens with 24 single lenses within, it has been successfully tested in the focusing and imaging modes both at the APS source [3] and at the laboratory setups using Cu K X-radiation from the rotating anode generator and microfocus MetalJet X-ray tube with a liquid-gallium jet as the anode using Ga Ka line. The lens has successfully reproduced the triangular object with the theoretical demagnification while the focusing of the 20 μm source was performed with the small deviation from the theoretical value.

The present study demonstrated that laser micro-fabrication technology provides a straight forward method for the fabrication of single-crystal diamond refractive lenses with large acceptance and high shape and surface (peak-to-valley roughness ~ 1μm) quality. Unique optical properties of diamond single-crystal lenses coupled with its excellent thermal qualities allows them to be applied as focusing, imaging and beam-conditioning elements at high-heat flux beams of today and future X-ray sources.

ADDITIONAL INFORMATION

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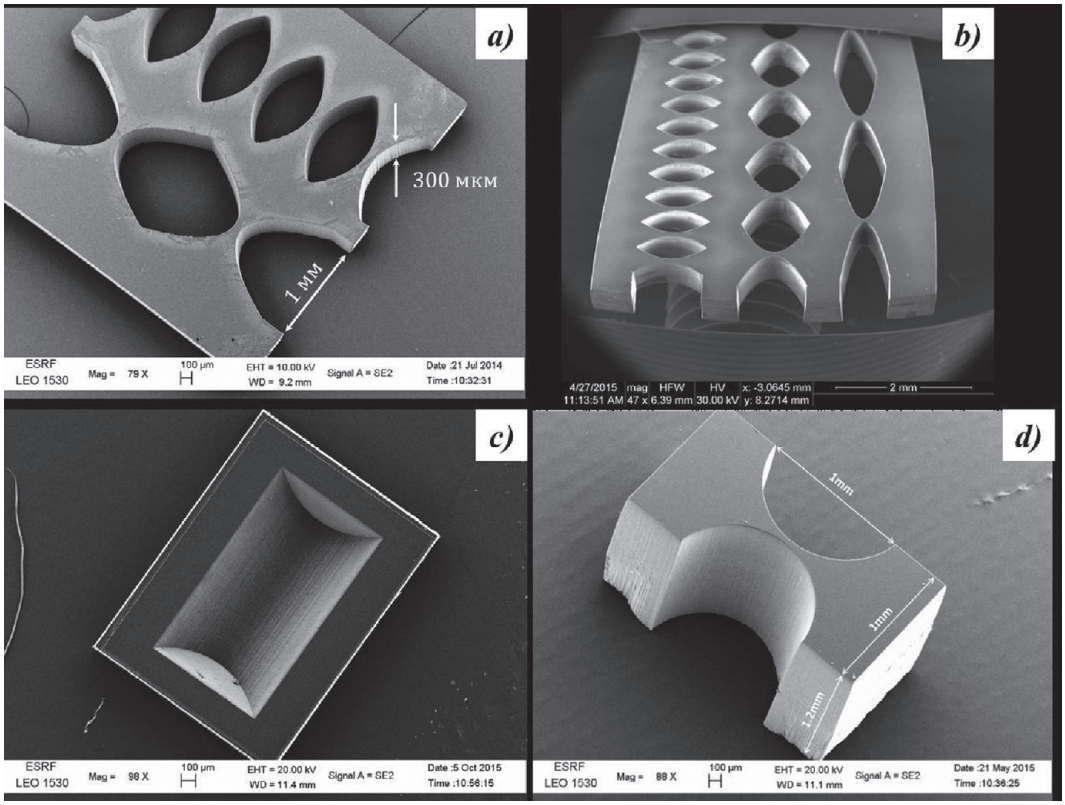

Figure 1. Planar refractive lenses from mono- (a,c,d) and polycrystalline (b) diamond

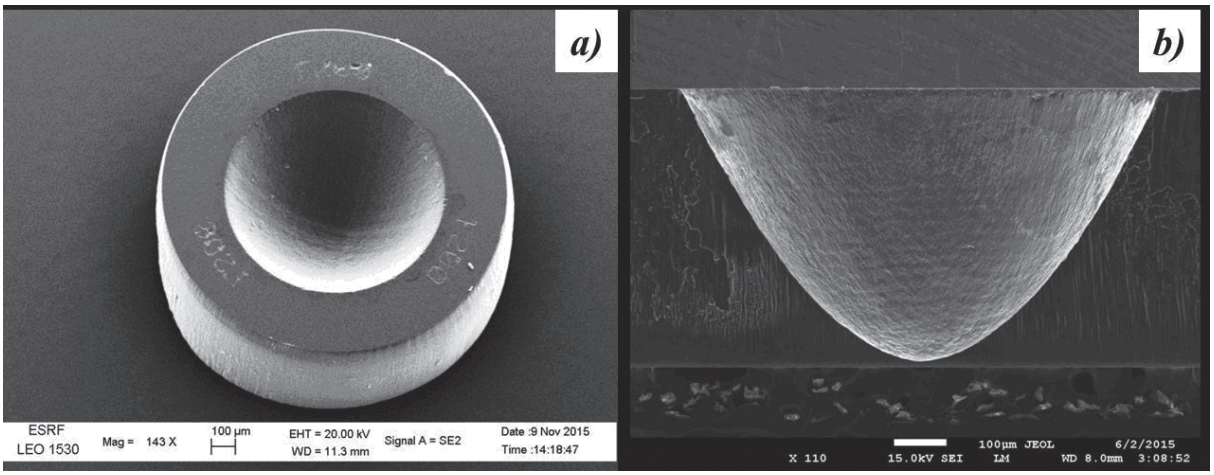

Figure 2. 2D parabolic single-crystal diamond refractive half lens (a) and its cross-section (b).

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Energy balance in divertor plasma detachment

SCIENTIFIC ORGANIZATION

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ABSTRACT

Divertor plasma detachment is analyzed from the viewpoint of energy and particle balance in the edge plasma. It is shown that volumetric recombination and impurity radiation losses are responsible for the transition to the detached plasma regime, whereas “momentum removal” plays although important, but auxiliary role providing conditions necessary for the first two to become efficient. A criterion of the local (on an isolated flux tube) detachment onset is studied for both pure and impurity-seeded plasmas.

KEYWORDS

Tokamak; Detachment; Impurity; Recombination.

ACKNOWLEDGEMENTS

This work was supported by the Russian Ministry of Education and Science grant No 14.Y26.31.0008.

SUMMARY

Plasma detachment from the divertor target promises efficient reduction of power loading on the targets in a tokamak-reactor. The experimental manifestation of detachment is a rollover, followed by a significant reduction, of the ion saturation current onto the target along with the increase of the fueling (gas puffing) rate. Original theoretical studies of this phenomenon lead to considering “momentum removal” – that is, some force acting on the plasma along the magnetic field – in the scrape-off layer (SOL), producing a drop of the plasma pressure between the mid-plane (“upstream”) and the target (“downstream”), as the principal cause of detachment. Although the reduction of the pressure near the target, accompanied by the decrease of the plasma temperature there, implies the reduction of the particle flux to the target, the story is not that simple. The flows in the edge are sustained by the sources and sinks of particles and the pressure profile adjusts itself to ensure the required flow pattern that can be far from the simple, laminar flow from upstream to downstream. Particle balance in the detaching plasma was considered in [1] where the volumetric recombination of the ions and electrons was identified as the mechanism responsible for the detachment. Globally, this balance means the equality of the fueling and pumping fluxes, since ionization and recombination do not affect the total particle content in the system. However, these flows are orders of magnitude lower than the recycling ones, so they can hardly affect the plasma state directly, controlling the particle content (or the plasma density) instead. The recycling fluxes depend in turn on the power available for ionization and recombination of the particles. Therefore, it is natural to consider the detachment process from the viewpoint of power balance, taking the particle content in the edge as the parameter characterizing the density.

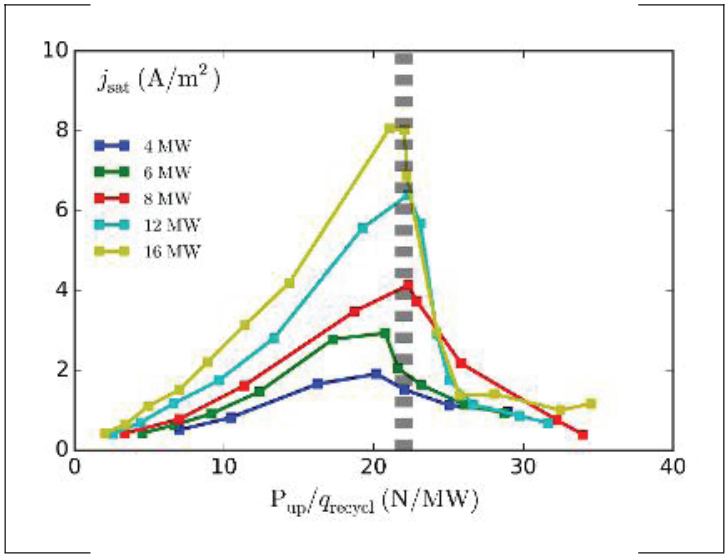

Fig. 1. j_{sat} vs. the P_{up}/q_{recycl} ratio for different power input to the SOL. DIII-D-like configuration, pure deuterium plasma.

This paper presents the results of theoretical and modelling analyses of the role of power balance in the recycling and recombining plasmas, following the approach of [2]. On the modeling side, the SOLPS4.3 code suite [3] was applied to a simplified geometry model built around a DIII-D-like magnetic equilibrium. In particular, the ratio of the plasma pressure upstream to the power flux entering the recycling region as the principal parameter controlling the j_{sat} rollover is identified in the theory and confirmed by modelling, Fig. 1. The results show that volumetric recombination and the power loss with

radiation from impurities are indeed directly responsible for detachment, whereas the “momentum removal” plays a secondary, although important, role in providing the conditions for these processes.

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ADDITIONAL INFORMATION

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Bright X-Ray Sources from Laser-Driven Nanostructured Plasmas

SCIENTIFIC ORGANIZATION

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ABSTRACT

As the laser technology continues its spectacular development, ever higher field intensities and power levels become accessible in laboratories. The laser pulse quality is greatly improved so that fine structured targets maintain their structure till the main pulse arrival. This opens new and unexpected possibilities for laser-plasma engineering towards new physics.

KEYWORDS

Plasma simulation, laser-plasma interaction, x ray sources

SUMMARY

As the laser technology continues its spectacular development, ever higher field intensities and power levels become accessible in laboratories. The ELI project opens new horizons for laser applications in ultra-bright sources of short wavelength radiation. At the same time, the laser pulse quality – like the contrast ratio – is greatly improved so that fine structured targets maintain their structure till the main pulse arrival. This opens new and unexpected possibilities for laser-plasma engineering towards new physics.

In the talk, we consider laser pulse interaction with nano- and micro-structured targets like nano-grass [1] and micro-channels [2] in the intensity range 10^{18}-10^{20} W/cm^2. At intensities higher than 10^{22} W/cm^2, the radiation damping force becomes important and can exceed the Lorentz force acting on an electron [3]. The g-ray emission is then the major channel of laser energy absorption [4].

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The influence of the frequency modulation parameters on the stability of CPT based atomic clock

SCIENTIFIC ORGANIZATION

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ABSTRACT

This paper investigates the influence of frequency modulation parameters on the stability of the atomic clock based on the effect of coherent population trapping in 87Rb vapor using the D1 transition. Research carried out for the two optical cells, one of which had antirelaxation cover, and the other had not. It was obtained the dependence of the stability of an atomic clock by frequency modulation parameters for each cell. The optimal parameters for two different cells were about the same. The stability for the coated cells in 1 second was 3x10^-11, and for the uncoated cell 1.5x10^-10.

KEYWORDS

Atomick clock, Frequency standard, Coherent Population Trapping, CPT

ACKNOWLEDGEMENTS

“MESRF №2014/139 pr №825, RSCF №16-12-10147”

SUMMARY

In recent years, many groups around the world have been actively studying the effect of coherent population trapping (CPT) in alkali metals and the related to its effect of electromagnetically-induced transparency (EIT). The effect of CPT consists in the studied medium atoms falling into the so-called ‘dark’ resonant state when pumped with a bi-chromatic optical field with the frequency difference close to that of the hyperfine splitting[1]. Atoms occupying this state cease to interact with the optical field, leading to observation of EIT. CPT resonances occurring in alkali metal atoms are known for their high quality factor of ~10^8[2], thus allowing their application as a quantum discriminator in frequency standards[3] and magnetometers[4]. For locking in the frequency of a quartz oscillator to the reference CPT resonance, the frequency difference of the bi-chromatic field around the resonance is modulated and a feed-back system with a lock-in amplifier is used. One of the advantages of this method is the possibility of noise filtering in the measurement system at frequencies not immediately adjacent to the modulation frequency[5]. Given the fact that the noise intensity is reduced as the frequency rises, selection of higher modulation frequency leads to lower noise level in the feedback system, thus improving the device performance. However, higher frequencies introduce a number of effects related to a finite time of excitation and relaxation of the coherent ‘dark state’.

This paper describes an experimental optimization of the feedback system in a 87Rb CPT based clock which employs a small cube glass cell with and without antirelaxation coating. The feedback loop is implemented by superimposing low rate frequency modulation (FM) on the microwave drive signal to the diode laser thereby enabling to probe the atomic vapor using the FM spectroscopy scheme. Classical FM spectroscopy employs only one FM modulated field. The properties of the demodulated signal for this case have been analyzed and measured. However when FM spectroscopy is used in CPT based clocks (where the interacting fields are the side bands of a directly modulated diode laser), each spectral component carries its corresponding FM side bands. The signature of the CPT process on the demodulated signal is consequently different than in the classical case. This difference which may be subtle has nevertheless a profound effect on the sensitivity and SNR of the error signal feeding the feedback loop. This is demonstrated in the experiments we describe here on which yield sets of FM parameters (FM modulation frequency and amplitude) that ensure optimum. Our experimental studies of the optimal FM parameters for CPT resonance formation were conducted on the installation schematically depicted in Fig. 1.

The injection current of a single-frequency vertical-cavity semiconductor laser pump was modulated at the frequency of 3.417 GHz generated with a frequency synthesiser Phase Matrix 10 GHz. This led to emergence of two side components

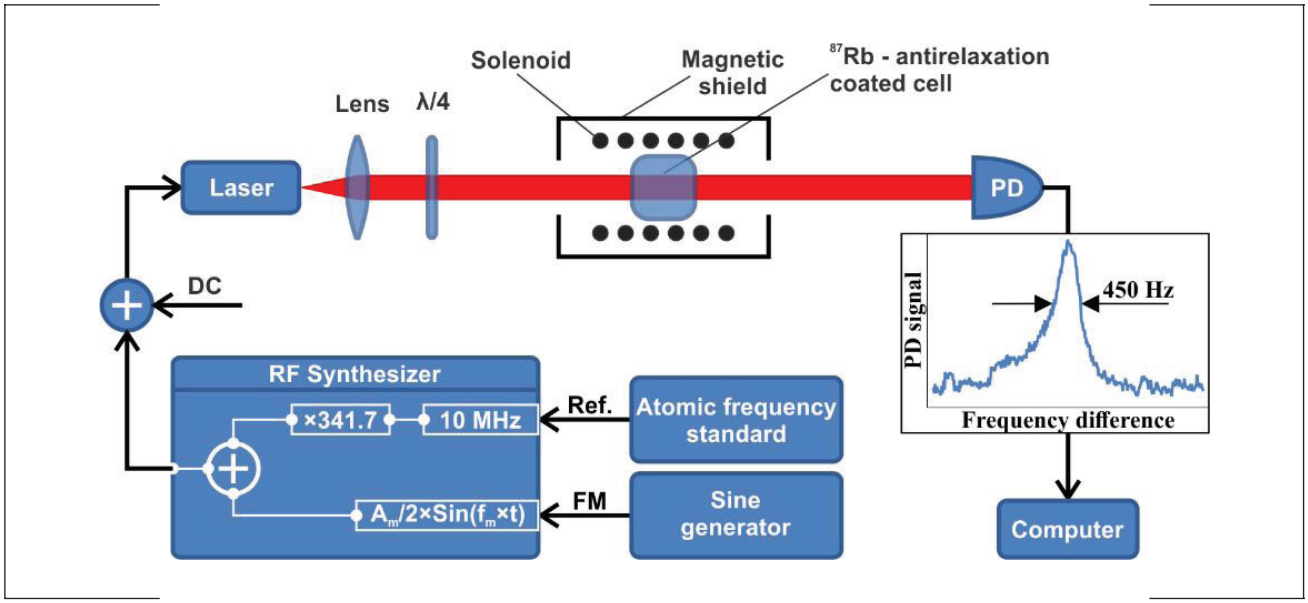


Fig. 1. Diagram of the experimental installation

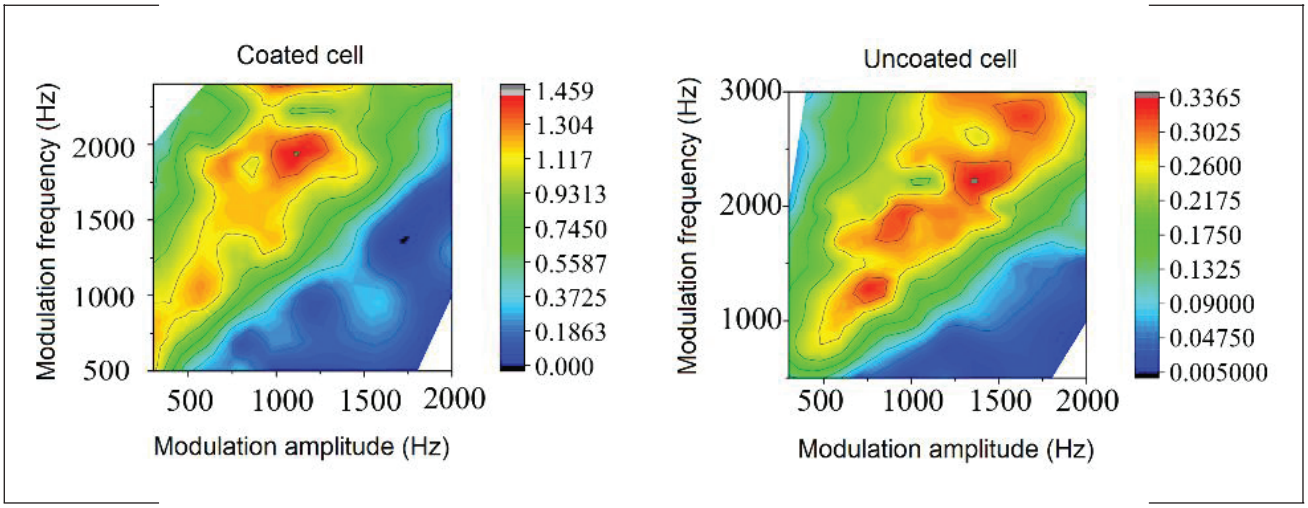
in the laser radiation spectrum detuned from the central peak by ± 3.417 GHz. A 10- MHz reference signal was provided by a rubidium atomic clock with relative instability of 10^–12/t. The frequency difference between the side components of the laser radiation corresponded to the frequency of the transition between the levels of hyperfine splitting of the fundamental state of 87Rb. To create a CPT resonance, the frequency difference between the side modes was modulated at a frequency that could be adjusted in the range of 300–2000 Hz, the modulation amplitude was adjusted in the range of 500–3000 Hz . The pumping radiation was then guided into an optical cell filled with 87Rb vapour. The intensity of the laser radiation passed through the cell was registered by a photo-detector with a 100-kHz bandwidth. In order to eliminate any external magnetic field, the optical cell was placed inside a three-layer magnetic shield. Both the pump laser and the optical cell were thermostabilised and their temperature instability did not exceed 10–3 °C. The power of the laser radiation entering the optical cell was 50 uW.

For each set of parameters measured by the change of the error signal at 10 Hz offset from the resonance. It was found that the error signal values are normally distributed. The magnitude of the standard deviation of the error signal was used as the amplitude of the noise

The result of this study is obtained according to the sensitivity of the feedback system for different cells. The dependency of the feedback loop sensitivity on modulation parameters for both cells shown in Fig. 2

It was found that despite the large difference in the width of the resonances best stability is achieved for all cells at approximately the same modulation parameters: amplitude and frequency of 1 kHz to 2 kHz. The best stability achieved at the maximum sensitivity of the feedback system is as follows: the coated cell - 3 x 10^-11; uncoated cell - 1.5 * 10^-10.

Fig. 2. Measured feedback system sensitivity for coated and uncoated cells



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High resolution heterodyne spectroscopy for studies of planetary atmospheres

SCIENTIFIC ORGANIZATION

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ABSTRACT

Heterodyne receivers are widely used in radio and microwave astronomy due to high sensitivity and unprecedented spectral resolution. Recent progress in semiconductor lasers and fiber optics has made it possible to expand heterodyne method to shorter wavelengths, including near-infrared spectral range. High resolution spectral radiometry in the fundamental ro-vibrational bands of atmospheric species provides a unique opportunity to detect minor components at ppt level, as well as to implement direct Doppler wind velocity measurements.

KEYWORDS

Planets, atmospheres, heterodyne, spectroscopy, infrared.

ACKNOWLEDGEMENTS

This work is supported by the Russian Science Foundation grants #16-12-10559 and #15-12-20040.

SUMMARY

We present a review of activities of the Applied Infrared Spectroscopy lab (AIRS) on high resolution heterodyne spectroscopy targeting sensitive studies of structure, composition, and dynamics of planetary atmospheres. Heterodyne method allows for unprecedented spectral resolution $\lambda/\delta\lambda \approx 10^8$ and signal-to-noise ratio close to the quantum limit. Its implementation in ground-based astronomy by several research groups in the US, Germany, and Japan has already provided valuable information about dynamics and composition of the atmospheres of terrestrial planets. New ideas implemented at AIRS resulted in the development of a series of instruments whose scientific objectives vary from greenhouse gas monitoring to *in situ* sounding of the Martian atmosphere from landing platform in the near-infrared spectral range by direct Sun observation. In addition, a novel instrument for ground-bsed astronomy is being developed. The instrument employs quantum cascade lasers as heterodyne and broadband mixer based on superconducting hot electron bolometer with optical antenna. Coupling local oscillator with the signal received from a telescope is provided by a single mode fiber coupler based on fused halcogenide optical fiber. Future development will allow to implement these technologies and engineering solution onboard Earth orbiting satellites and interplanetary spacecraft.

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Resonant elastic driving of magnetization precession in ferromagnetic nanogratings

SCIENTIFIC ORGANIZATION

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ABSTRACT

We study the interaction of magnetization and hypersound surface elastic waves optically excited in a planar ferromagnetic nanogratings. We demonstrate the long living magnetization precession at resonant conditions when the ferromagnetic resonance frequency controlled by external magnetic field matches the frequency of surface elastic wave determined by the grating parameters. This resonant elastic driving of precession occurs even if applied external magnetic field totally suppressed the excitation of precession in non-patterned area of a film.

KEYWORDS

Ultrafast magnetoacoustics, ferromagnetic nanostructures, magnetoacoustic resonance.

ACKNOWLEDGEMENTS

The work was supported by the Russian Science Foundation (Grant No 16-12-10485).

SUMMARY

We report the ultrafast experiments with planar metallic ferromagnetic nanostructures, in which we realize the resonant driving of magnetization precession by surface elastic waves of hypersound frequencies (10^{10} Hz). This work continues our ultrafast magneto-acoustic studies started in 2010 [1] and demonstrates ability to spatially localize the magnetization precession by its coupling with high-frequency coherent elastic excitations in an optically excited ferromagnet.

The planar nanostructures for our studies were produced by focus ion beam nanolithography on a film of ferromagnetic galfenol ($Fe_{0.81}Ga_{0.19}$) of 100-nm thickness grown on (100)-GaAs substrate. The grooves of 40 nm depth were etched to from a periodic grating. Several structures of 5x5-microns lateral size with different parameters were produced: groove' direction was either parallel to [100] or [110] crystallographic direction, the groove width/grating period were 40/150 and 50/190 nm.

At the experiment performed in a conventional pump-probe scheme, we use femtosecond pulses of an Yb:KGW regenerative amplifier (1030 nm wavelength, 200 fs pulse duration, 5 KHz repetition rate) to excite and detect the magneto-elastic response. The pump pulse was focused to the spot of 100 microns (excitation density was up to 20 mJ/cm^2) and, thus, covers both the patterned and non-patterned parts of the film. The linearly polarized probe pulse focused by means of 50x microobjective to the spot of submicron size allows selective detection of the magneto-elastic kinetics either from the patterned structure or the non-patterned film area. We monitor the rotation of the probe polarization plane (magneto-optical Kerr effect) as a function of delay between the pump and probe pulses.

The non-patterned film demonstrates a typical response on optical excitation with an oscillating Kerr rotation signal, which reflects the precession of magnetization excited due to the ultrafast changes of the magneto-crystalline anisotropy (MCA). The dependences of the precession frequency (i.e. the ferromagnetic resonance frequency) and amplitude on direction and strength of external magnetic field, **B**, are typical for a metal ferromagnetic film and determined by the MCA. At **B**||[100] we observe the magnetization precession with frequency linearly increasing with *B* and with weak nonmonotonic field dependence of the precession amplitude. At **B**||[110] we detect no excitation of the magnetization precession. The same results in non-patterned galfenol films were obtained in our previous ultrafast magneto-optical experiments performed without submicron spatial resolution [2].

The main result of the present work is the drastically different magnetization response observed in the patterned structures. In the structures with the grating oriented along [100] crystallographic direction at **B**||[110] we, contrary, observe

the long-living (up to 3 ns) precessional response. The detected frequency (15 GHz for the grating period of 150 nm) is independent of *B,* while the amplitude demonstrates strong field dependence. The sharp maximum of the precession amplitude is achieved at *B*=150 mT, which corresponds to the ferromagnetic resonance frequency of 15 GHz. Such a behavior demonstrated before in our experiments with ferromagnetic nanolayer embedded into phononic Fabry-Perot resonator indicates the resonant driving of magnetization precession by localized elastic excitations [3]. The surface acoustic wave (SAW) with the wavevector determined by the grating period is optically excited in a patterned structure. Due to large depth of the grating, the SAW velocity in a patterned area is significantly lower than in non-patterned one [4] and, thus, the SAW remains localized. This results in resonant driving of the magnetization precession when the resonant conditions controlled by external magnetic field are fulfilled.

This research is result of collaboration between the Laboratory of the Physics of Ferroics “Ferrolab” of the Ioffe Institute (Anastasya Rudkovskaya, Alexey Salasyuk and Alexey Scherbakov), the Institute of Nanotechnology for Microelectronics of the Russian Academy of Science (Polina Nekludova, Sergey Sokolov and Andrey Elistratov), the Lashkaryov Institute of the National Academy of Science, Ukraine (Boris Glavin) and the University of Nottingham, UK (Andrey Akimov and Andrew Rushforth).

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Detecting nuclear polarization dynamics by spin noise spectroscopy

SCIENTIFIC ORGANIZATION

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ABSTRACT

Spin noise spectroscopy (SNS) is a rapidly developing tool of non-perturbative magnetooptic investigations. The lastest achievements of this technique reveals its new magnetometric potential. This research demonstrates the possibility of direct measuring of the magnetic fields acting upon electron spin-system of an n-GaAs layer, such as the Overhauser field created by optically oriented nuclei.

KEYWORDS

Spin noise spectroscopy, magnetooptics, paramagnetic resonance, semiconductors.

ACKNOWLEDGEMENTS

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SUMMARY

Spin noise spectroscopy (SNS) gained a lot of popularity in the last decade, when it was proven to be a highly efficient method of non-perturbative exploration of charge carrier dynamics and magnetic resonance in semiconductor systems. The fluctuation-dissipation theorem manifests the possibility of detection of linear sus-

ceptibility resonances in the medium by registration of the noise spectrum of this system. As applied to magnetic resonance spectroscopy, this principle can be realized by detecting fluctuations of the Faraday rotation of the linearly polarized probe beam passing through a transparent paramagnet. The detected noise signal is proportional to fluctuations of the medium magnetization. In the presence of magnetic field which is perpendicular to the light propagation axis the Faraday rotation noise spectrum reveals a peak at the magnetic resonance frequency corresponding to precession of spontaneous fluctuations of the spin ensemble at the Larmor frequency. In the absence of absorption in the sample the system remains in thermodynamical equilibrium, so the method can be regarded as essentially non-perturbative. The features like the possibility of three-dimensional tomographic measurements; no necessity for conventional ESR microwave equipment; widely extendable (up to hundreds of GHz) detection range; experimental simplicity are the most noticeable advances of this method among the others.

Due to very small magnitude of spontaneous magnetization fluctuations, spin noise spectroscopy necessitate the highest polarimetric sensitivity, which is fundamentally limited (for classical light emitters) by photon flux shot noise level. Higher sensitivity of measurements in this limit can be achieved by the increase of the probe light power density, which leads to increase of nonlinear light-matter interaction effects. In such conditions the experiment cannot be considered as non-perturbative, however nonlinear SNS experiments brings a lot of information about optical and magnetic effects in a semiconductor structures.

In the present work we uncover the magnetometric potential of the SNS. It is based on the known fact that the electron spin noise (SN) spectrum at arbitrary orientation of the external magnetic field generally reveals two components. The one of them is centered at zero frequency and reflects fluctuations of the longitudinal magnetization, while the other is centered at Larmor frequency and results from fluctuations of the transverse magnetization. Its magnitudes ratio is determined by mutual orientation of the light beam and magnetic field and therefore can be used to monitor direction of the effective magnetic field acting upon the spin system. In our work we show that SNS can be used for direct detection of the Overhauser field of the nuclei, optically oriented by the high-power elliptically polarized probe beam.

Host lattice nuclear spins occupy a special place among spin systems in semiconductors. Its exceptional robustness to effects of environment opens up prospects to use nuclear spins for information processing. On the other hand, they play major role in electron spin dynamics and decoherence. Mechanisms of the nuclear spin relaxation in n-type semiconductors, even in the best studied like GaAs, remain rather poorly understood. Weak interaction of nuclear spins with light significantly complicates direct optical studies of nuclear spin dynamics. In the present work, we involve SNS to investigate nuclear spin dynamics in n-doped semiconductors. The technique is applied to *n*-type GaAs layers embedded into a high-finesse microcavity. We show that nuclear spins can be optically polarized by the circularly polarized beam due to the residual absorption of the sample. The detection is achieved via Kerr rotation spectra recorded with time resolution of several seconds. A shift of the electron precession peak with respect to its unperturbed position, when nuclei are not polarized, is a direct measure of the Overhauser field B_N created by optically cooled nuclei. SNS spectroscopy provides a direct measurement of B_N with time resolution given by the SN spectrum acquisition time. The proposed method is applied to both metallic and insulating samples, revealing full potential of this technique, which allows to investigate nuclear spin relaxation in the presence of either donor-bound localized electrons, or mobile Fermi-edge electrons.

In addition to the retarded response, ascribed to nuclear system polarization buildup and decay, SN spectra also reveals an instantaneous shift of the precession peak and appearance of the non-magnetic component, similar to appearance of the additional longitudinal magnetic field. This effect is attributed to ac Stark effect acting upon spin system in the electromagnetic field of elliptically polarized high power density light. The effect is also illustrated by corresponding SNS measurements and described in more detail in the recent work of the team of contributors.

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5 bit current steering low power DAC for threshold voltage adjustment

SCIENTIFIC ORGANIZATION

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ABSTRACT

In this paper a low power integrated circuit of 5 bit current steering DAC is presented. The proposed DAC is integrated to prototype the readout channel for muon chamber in international CBM experiment at accelerated facility FAIR. DAC was implemented with an area of 0.019 mm2 using UMC MMRF 180 nm CMOS process. This DAC has ultralow power consumption - 25μW. The measured maximum differential nonlinearity (DNL) is 0.25 LSB (less significant bit), integral nonlinearity (INL) is 0.2 LSB. In this paper the main steps of design flow, simulation and measurement results are presented.

KEYWORDS

DAC, ASIC, readout channel.

ACKNOWLEDGEMENTS

This work was supported by Grant No. 14.A12.31.0002, issued in 2013 by the Russian Federation Ministry of Education and Science according to the RF Governmental resolution No 220.

SUMMARY

A prototype readout channel for CBM experiment was designed and manufactured by the UMC 180 nm CMOS technology. The structure of the channel is shown in figure 1 [7]. The analog part of channel includes a preamplifier, shaper, DAC, comparator and ADC. The comparator generates the start of conversion signal for ADC, when the signal from detector comes to the input of comparator. It is necessary to exclude false triggering by noise, so the threshold voltage of comparator must be adjustable. One of the most wide-spread methods of adjusting voltage is doing that by a digital to analog converter. Because of the large number of channels in one chip, the proposed DAC must be low power and efficient by area on chip. Also the threshold voltage adjustment must be quite accurate, so the proposed DAC must have a high linearity. Also the threshold voltage adjustment does not require a high speed of conversion. So the following requirements were formulated for the proposed DAC and presented in table 1.

Fig. 1. Prototype readout channel structure

TABLE 1

Requirements for the proposed DAC

Technology	UMC 180 nm
Supply voltage	1.8 V
Resolution	5 bits
Power consumption	<100 μW
INL	<1 LSB
DNL	< 1 LSB
Area	< 0.03 mm^2

DAC IMPLEMENTATION

Design flow of the proposed DAC consists of five steps:

1. Design of schematic.
2. Simulation
3. Design of layout
4. Verification and parasitic elements extraction
5. Simulation of verified schematic

The proposed DAC has a binary weighted architecture. This architecture was chosen because there is a special buffer before comparator, that produces a differential signal and adjust the threshold voltage proportionally to input current. Also there are only five current sources and a bias block, without any special buffers, so that the architecture is well suited for small resolution because of a low power consumption and small area on chip. Because of current sources, which are made on transistor level without resistors, that architecture provides a high linearity of output current.

The proposed DAC consists of a biasing circuit, current matrix and output stage. The DAC structure is presented in figure 2. The schematic of DAC was designed in the Cadence Virtuoso schematic editor. The biasing circuit produces bias voltages for the correct work of current matrix. Schematic of the bias is shown in figure 3. The main part of the DAC is a current matrix. It consists of five current sources.

Fig. 2. DAC structure Fig. 3. Biasing circuit

One of the most important parameters of the current source is linearity. Transistor mismatch in current sources causes the nonlinearity of the DAC [1]. Increasing the area of transistors in current sources reduces nonlinearity [2], so the main transistors must have the maximum available channel length in the technology (50 μm). The series combination of current producing transistors M1 and M2 is implemented for the same unit current to achieve larger area and consequently a better matching and higher linearity. Another thing, which improves DAC nonlinearity, is a high output impedance of each current source. To increase output impedance a cascode transistor has been used. Because of the large area of main transistors M1 and M2, the output impedance is reduced. Since the cascode transistor does not effect the output current, it will not contribute any mismatch. So the cascode transistor must have the minimum available channel length in the technology (180 nm). Also, to compensate the reduction of output impedance associated with the large current producing transistors, gain boosting has been used to increase the output impedance in each current cell [3]. To achieve enough output impedance the feedback path should be designed. The schematic of current source is presented in figure 4.

Fig. 4. Current source schematic

SIMULATION

The main characteristics were simulated in Analog Design Environment (ADE) by using Monte-Carlo analysis. Since the designed DAC is static, the main static nonidealities, such as differential nonlinearity (DNL), integral nonlinearity (INL), gain error and offset, were simulated. DNL(k) is a vector that quantifies for each code k the deviation of this width from the “average” width (step size) [3]. DNL(k) is a measure of uniformity, it does not depend on gain and offset errors. Scaling and shifting a transfer characteristic does not alter its uniformity and hence DNL(k). DNL calculation [3], [4], [5]:

(1)

Integral nonlinearity is the maximum between transfer characteristic and a straight line drawn through the endpoints from each relevant point of transfer characteristic. Just as with DNL, the INL of a converter is by definition independent of gain and offset errors. INL calculation [3], [4], [5]:

(2)

Offset is the deviation of bottom endpoint from its ideal location [3]. Gain error is the deviation of top endpoint from its ideal location with offset removed [3]. Simulation results are presented in table 2. The results of Monte-Carlo simulation of transfer curve is shown on figure 6. The results of noise analysis is presented in figure 7.

TABLE 2

Simulation results

Power consumption	25 μW
INL	<0.2 LSB
DNL	< 0.15 LSB
Gain error	0.5 LSB
Offset	0.05 LSB
LSB	200 nA

Fig. 6. Monte-Carlo results of transfer function

Fig. 7. Noise simulation of transfer function

Layout of the proposed DAC was designed in Cadence Virtuoso Layout XL and verified by using Calibre tool of Mentor Graphics Company. The chip was fabricated by UMC 180 nm CMOS technology available through Europractice foundation. The area of the designed layout is 190 by 100 μm2. Experimental results were obtained by using following instruments: pulse function arbitrary generation by Keysight 81160A, at laboratory conditions by usage Agilent oscilloscope DSO9104H, probe station of Cascade Michrotech. For DNL, INL, gain error and offset calculation Mathlab program package was used. Figure 8 and figure 9 show DNL and INL respectively, the maximum DNL and INL are 0.25 LSB and 0.2 LSB respectively. Offset error is 0.7 LSB, gain error is 3.5 LSB.

Fig. 8. Differential nonlinearity Fig. 9. Integral nonlinearity

TABLE 3

Characteristics of the proposed DAC

Technology	UMC 180 nm
Supply voltage	1.8 V
Resolution	5 bits
Power consumption	25 μW
INL	0.2 LSB
DNL	0.25LSB
Area	< 0.019 mm^2
Gain error	3.5 LSB
Offset error	0.7 LSB

Conclusion

A 5 bit current steering low power area efficient DAC has been designed in UMC 180 nm CMOS technology. Main specifications are presented in table 3. The DAC was designed in binary weighted architecture. To reduce nonlinearity two voltage driven transistors with maximum channel length were used in each current source. The power consumption is 25 μW at 1.8 V power supply. Presented DAC was integrated as a building block into prototype readout channel for CBM experiment being currently under construction at FAIR. This work is done in full accordance with grant No. 14.A12.31.0002. At the same time advanced computer equipment and microelectronic CADs and also control and measuring equipment, deployed in the laboratory under the grant, were used.

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ADDITIONAL INFORMATION

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Generation of gamma-rays and hard X-rays by intense ultra-short laser pulses interacting with foils: normal and oblique incidence

SCIENTIFIC ORGANIZATION

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ABSTRACT

We theoretically and numerically investigate the process of gamma-ray generation when ultra-intense laser pulses (with a0 ~ 100) hit the foil. We consider both normal and oblique incidence. The theoretical approach is based on a self-consistent model of dynamics of the thin surface electron layer and gives properties of gamma-ray radiation that well correspond to our particle-in-cell simulations. The numerical approach gives us possibility to optimize the interaction scheme and determine the parameters of most efficient gamma-ray generation.

KEYWORDS

Ultra-intense laser pulses, oblique incidence, gamma-ray generation.

ACKNOWLEDGEMENTS

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SUMMARY

During the last 30 years an outstanding progress in ultrashort-pulse laser technology has been achieved. This allowed one to obtain ultra-high values of electromagnetic fields (so electrons and even ions become relativistic is such fields) in the laboratory. The maximum attainable laser intensity nowadays is of the order of 10^{22} W/cm^2. That results in near-QED regimes of laser-matter interaction.

Interaction of ultrashort laser pulses with different targets is expected to be a very promising mechanism of electron and ion acceleration, and generation of high-energy quanta (hard X-rays and gamma-rays). This topic is heavily studied nowadays: for example, use of intense laser pulses for generating bright gamma-ray flashes has been showed in the papers of Nakamura et. al. [1] and Nerush et. al. [2] At the described laser intensities the electrons in the target are quickly accelerated up to ultra-relativistic velocities and begin to emit gamma-rays and hard X-rays very efficiently. The maximum achieved conversion efficiency of the laser pulse energy into the energy of hard photons is tens of percent. However, the properties of the gamma-ray flash are usually much worse than what is obtained with help of traditional sources (i.e. radioactive sources or based on Compton backscattering) and there is still space for optimization of the laser-matter interaction scheme. For example, the effect of use of oblique-incident laser pulses is not much investigated.

To our knowledge, there is lack of understanding of what happens during laser-foil interaction and how gamma-quanta are generated. There are several theoretical models but most of them can’t help to know the Lorentz factor of the electrons

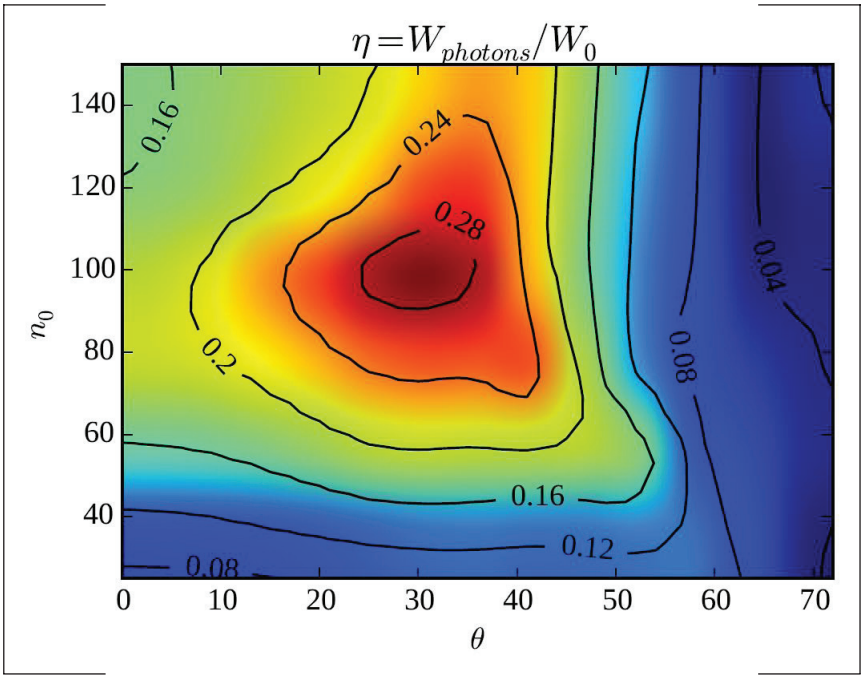

Figure 1. Gamma-ray generation efficiency as a function of plasma density and angle of incidence.

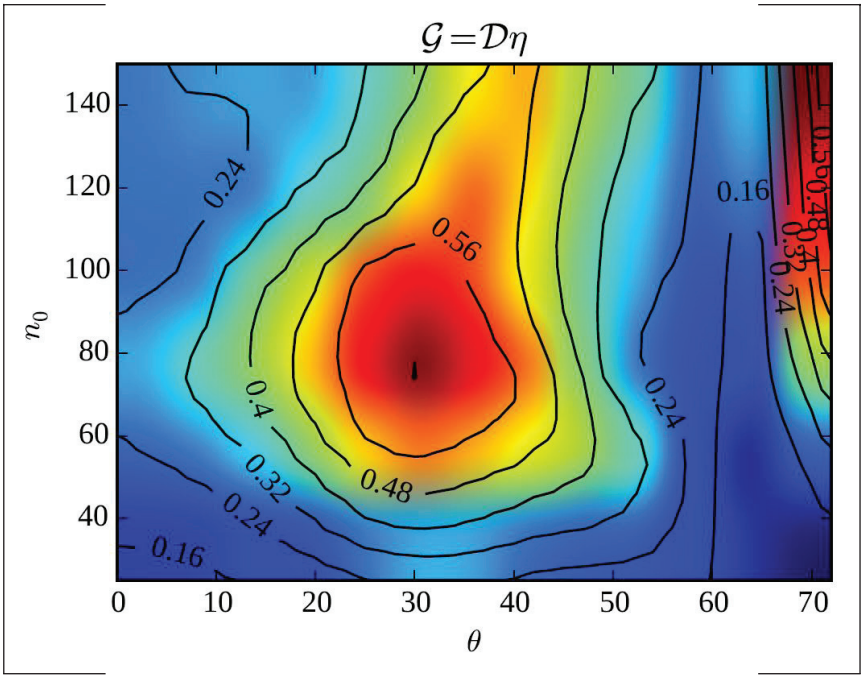

Figure 2. Gain *G* as a function of plasma density and angle of incidence.

and they can be barely used for estimating the gamma-ray radiation pattern. In the current work we try to explain the interaction process by using a theoretical model of thin surface electron layer which almost reflects the falling laser pulse. In the framework of this model, the layer is moving under both electric and magnetic laser fields, the change separation fields from the ions and the radiation reaction force (which should be also taken into consideration at our laser field intensities). The electron layer dynamics can be described with self-consistent equations (more detail one can find in our paper [3]). After solving the equations of electron layer dynamics we can govern the trajectory of the layer and the electrons Lorentz factor (this is the most important feature of the model being used). This model can be also applied to the case of oblique incidence by performing a Lorentz transform into the appropriate reference frame (see [4] for more detail). We show that the model can be still applicable for the case of oblique incidence for some angles. The modeling of the plasma surface showed good correspondence with the numerical simulation results.

We also show that in the case of oblique incidence the gamma-ray generation efficiency increases. In order to optimize the interaction parameters (the incidence angle, the target density) we have carried out a series of particle-in-cell (PIC) 3D numerical simulations. This allowed us to determine the optimal parameters that lead to the best efficiency – the optimal incidence angle is 30° and the target density is about 2 times lower than the dimensionless laser field amplitude a_0 (see Fig. 1). In our numerical experiments *a0* was of the order of 100. If to define gain *G* as the product of gamma-ray generation efficiency and the radiation pattern directivity (i.e. the ratio between the maximum value in the radiation pattern and the average value), we can see that high G region also lies near the angle of 30° (see Fig. 2), but the optimal plasma density becomes lower.

In the fig. 2 we can also see that at high angles (approximately 66° and higher) the gain increases. In this region the generation efficiency is not very high but gamma-rays have very narrow radiation pattern which may be useful for different applications. We also discuss theoretical reasons for qualitative change in the shape of the radiation pattern.

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Hydrological cycle in the Martian atmosphere general circulation numerical model MAOAM

SCIENTIFIC ORGANIZATION

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ABSTRACT

We consider the numerical modeling problem formulation of the Martian atmosphere general circulation using the meteorology primitive equations approximate solution. We use model MAOAM (The Martian Atmosphere: Observation and Modeling) with a spectral dynamic kernel KMCM (Kühlungsborn Mechanistic general Circulation Model) as a basic model. The stable hydrological cycle modeling was achieved during a Martian year.

KEYWORDS

Water cycle, numerical modeling, atmosphere, climate, general circulation model, MAOAM, advection, ice sedimentation, water phase transformation, surface water exchange.

ACKNOWLEDGEMENTS

Work has carried out in the Laboratory of Infrared Spectroscopy of Planetary Atmospheres High Resolution of the Moscow Institute of Physics and Technology (State University) supported by the grant №11.G34.31.0074 of the Ministry of Education and Science of the Russian Federation.

SUMMARY

We consider the numerical modeling problem formulation of the Martian atmosphere general circulation using the meteorology primitive equations approximate solution. We use model MAOAM (The Martian Atmosphere: Observation and Modeling) with a spectral dynamic kernel KMCM (Kühlungsborn Mechanistic general Circulation Model) as a basic model.

Hydrological cycle model is one of the essential components in modern Mars atmosphere general circulation models, for which, in turn, an aerosol unit and surface physics unit have been required. Primarily we were supposed to develop three-dimensional advection scheme (transfer) of a passive tracer atmospheric flows to create these units in such a way that numerical scheme hasn't lost conservatism with allowance water-ice phase transitions. In addition, it was necessary to develop the scheme for energy and matter (water and carbon dioxide) exchange between the atmosphere and the surface, as well as the deposited ice influence on the planet's surface physical parameters such as albedo and thermal inertia.

We have achieved sustainable model accounts for several Martian years during the implementation of the objectives, while maintaining stable and conservative scheme. We have investigated the hydrological cycle dependence on the initial conditions (the water vapor latitudinal gradient) and on the model parameters such as the ice particles sizes in 4 bins with different dust core nucleation sizes, affecting sedimentation, surface albedo and thermal inertia. Also it is using special schemes for nucleation, particle grows and vertical turbulent water diffusion. One of the modeling arising tasks from the observed data is the South Pole clouds mass increasing in the summer on the South Pole and the tropical belt clouds mass reducing in the aphelion season. These results were obtained thanks to the model parameters selection and to the using of the spectral numerical scheme, which has a smaller numerical viscosity and therefore provides a more intense meridional circulation, compared with the previously used grid scheme.

ADDITIONAL INFORMATION

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The Wave Flow Effect on a Plane Boundary between Vacuum and an Optical Medium with a Quasi-Zero Refractive Index

SCIENTIFIC ORGANIZATION

Technological Research Institute of Ulyanovsk State University

ABSTRACT

Results of theoretical and experimental researches of new metamaterial with silver nanoparticles in a dielectric matrix are presented. The received metamaterial possesses small absorption and small refractive index. Formulas for reflective and refractive abilities of a layer with quasi-zero refractive index which correctly describe experimental spectra of reflection and a transmission of a layer are removed.

KEYWORDS

Experimental spectra reflection and transmission of the layer, Formulae for reflectivity and transmittance of the layer with a quasi-zero refractive index, Inhomogeneous boundary, Layer with a quasi-zero refractive index, Non-Fresnel reflection and refraction of light, Random refractive index

ACKNOWLEDGEMENTS

This work was supported by the Ministry of Education and Science of the Russian Federation in the framework of a state assignment, project №. 14.Z50.31.0015.

SUMMARY

Results of theoretical and experimental researhes of new metamaterial with silver nanoparticles in a dielectric matrix are presented. This metamaterial is synthesized on the technology developed by us, samples of coatings on glass, silicon and a surface of serially let out silicon solar elements by means of technology of pneumatic dispersion of nanosuspension are received. On the basis of experimental spectra of reflection and a transmission of layers from the metamaterial synthesized by us effects of an interference of light in thick layers, the enhanced optical transmission, a broadband optical antireflection of surfaces are found. The received metamaterial possesses small absorption and small refractive index. It is proved that the refractive index of metamaterial is a random variable and area of admissible values of refractive index of this metamaterial, smaller units, is determined by an arrangement of interferential minima in experimental spectra of reflection of a layer. Formulas for reflective and refractive abilities of a layer with quasi-zero refractive index which correctly describe experimental spectra of reflection and a transmission of a layer are removed. On the basis of the developed theory of optical properties of a composite layer with quasi-zero refractive index new effects such as localization of photons on layer border, focusing of light in a layer, a wave flow effect are predicted by light of a surface of a layer. It is shown that new material with quasi-zero refractive index can find broad application in science and equipment, for example, in optical instrument making, solar industry, quantum electronics.

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Mathematical modeling of nonlinear propagation of the signal in the multimode fiber-optic communication lines

SCIENTIFIC ORGANIZATION

Novosibirsk State University

ABSTRACT

The work presents the results of numerical simulation of nonlinear propagation of the signal in the multimode fiber-optic communication lines. The main objective of this investigation is to demonstrate the possibility of long-haul data transmission over multimode fiber link at a higher rate as compared to the modern lines of communication.

KEYWORDS

Numerical simulation, optical fiber, communication line, multimode fiber, Schrodinger equation, nonlinear optics.

ACKNOWLEDGEMENTS

The authors acknowledge financial support from the Ministry of Education and Science of the Russian Federation (14.B25.31.0003).

SUMMARY

Currently more than 99% of the global flow of information are provided by technologies of fiber-optic communication. The annual traffic growth already exceeds the growth of the transmission capacity, and in the nearest years, we may face the problem of the traffic volume exceeding the capabilities of data transmission technologies, if no new technology, providing a significant increase in the transmission capacity of communication lines, will be offered.

Using various digital signal processing methods and modulation formats the data transmission rate of several hundred Tbit/s over standart single-mode fiber was achieved. However, further increasing the capacity of the SSMF is difficult due to limitations of the operating range of fiber amplifiers, high requirements of the signal/noise ratio, restrictions on the power of the signal injected into the fiber.

The development of communication systems based on multi-mode fibers is considered as a promising way for solving the above problem. Multi-mode fibers allow an increase in the transmission capacity of optical networks at the expense of simultaneous transmission of signals through multiple modes of the fiber. The research of the data systems based on multimode fibers started recently, and most of the published works are devoted to the linear regime of the signal propagation which significantly reduces the area of applications of of such fibers. However, it is known that the main limitations of fiber links are the nonlinear effects in the optical fiber. Therefore, the objective of this work was to study the nonlinear propagation of signals in data transmission systems based on multimode fiber over long distances. This work was aimed at obtaining practically realizable multimode fiber communication systems based on numerical experiment.

The main method of research is the mathematical modeling, which currently is a powerful, and sometimes the only possible tool for the study of new generations of fiber-optic communication lines and optimization of existing fiber-optic links to the range of parameters in which physical experiment is not possible due to financial, time or other constraints.

In the course of the study, new models for mathematical modeling of the nonlinear propagation in a multimode fiber in conditions of strong and weak coupling were developed. Also it was developed a numerical algorithm based on finite-difference compact scheme of high order for the solution of the basic equations of mathematical models, which in some cases may be more effective than the split-step Fourier method, which currently is the main numerical methods used in nonlinear fiber optics . For numerical algorithm software complex for high-performance computing was developed.

In the present work we compared weak- and strong-coupling regimes. It was shown that with the growth of the number of modes the strong coupling regime

provides a lower level of BER than the weak coupling one. We also investigated the dependence of BER on differential group delay (DGD) between the modes. It was shown that performance increases with increasing DGD.

One of the main challenges of long-distance propagation in multi-mode fibers in weak-coupling regime is the complexity of MIMO receivers that used to equalize for mode coupling. We compared two types of multi-mode fibers to meet this challenge: MMF with low DGD and with compensated DGD (combining fiber sections with DGD of opposite sign). MMF with low DGD demonstrate better performance than fibers with DGD management for long-distance transmission.

Also, research and development of methods of coding and signal modulation formats applicable to multimode fiber-optic lines, which can significantly increase the data transfer rate and reduce transmission errors, were carried out in the work.

The selected line of research, certainly, is an important application and commercial problem. The study results allow us to determine the boundaries of the area of applicability of multimode fiber in modern communication systems and can become the theoretical basis for the development of recommendations and proposals for the design of future fiber-optic communication lines. The results will help to reduce the number of expensive components in the high-speed fiber-optic links and significantly increase the capacity of communication lines.

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Senior research scientis

Femtosecond laser writing in high-purity tellurite glasses

SCIENTIFIC ORGANIZATION

D. Mendeleev University of Chemical Technology of Russia

ABSTRACT

The nonlinear optical properties and femtosecond writing in high-purity zinc- and tungstate- tellurite glasses doped with molybdenum, lanthanum or bismuth oxides were studied. We determined Kerr nonlinearity coefficient with Z-scan technique. The highest non-linearity was obtained for bismuth oxide modified glasses. Series of tracks with decreased refraction index were recorded in the bulk of samples under wide range of pulse energies, repetition rates, and scan speeds.

KEYWORDS

Laser direct writing, tellurite glasses, nonlinear refrative index.

ACKNOWLEDGEMENTS

The study was supported by the Ministry of Education and Science of the Russian Federation (grant no. 14.Z50.31.0009) and by the Russian Foundation for Basic Research (15-43-02185).

SUMMARY

Glasses based on tellurium dioxide are characterized by low phonon energy and can be obtained with an extremely low 3d-transition metals and hydroxyl groups impurities content, that provides transparency in the near and mid infrared regions. At the same time, viscosity parameters, sufficient mechanical strength and high nonlinear refractive index make them a very attractive matter for bulk and waveguide devices.

We studied the nonlinear optical properties and femtosecond laser writing in high-purity zinc- and tungstate- tellurite glasses modified with molybdenum, lanthanum or bismuth oxides.

The glasses were produced by melting the oxides in gold or platinum crucibles inside a sealed silica chamber filled with purified oxygen. TeO_2, WO_3, MoO_3 fabricated in our laboratory by original techniques and commercial high-purity ZnO, La_2O_3, Bi_2O_3 were used for glass synthesis. The total content of the 3d-transition metals impurities in raw materials and in glasses did not exceed 1-2 ppm wt. High stability of glasses against crystallization was confirmed by DSC at a heating rate 10 K/

min and there were no thermal effects of crystallization and melting of crystals. The hydroxyl groups absorption at ~3 μm, being calculated from transmission spectra by the Beer–Lambert–Bouguer law equation, was as low as 0.001-0.01 cm^{-1} in the glass samples prepared.

Using Z-scan technique [1] we have experimentally determined Kerr nonlinear coefficient γ that characterizes refractive index change Dn due to response of electronic shells:

$$\Delta n = \gamma I, \qquad (1)$$

where *I* is a light intensity. The femtosecond laser beam was focused by a lens with focal distance of 250 mm. Beam waist radius in focal plane was of 50 microns. Laser operation wavelength was of 1030 nm, pulse duration was about 180 fs, and repetition rate equaled to 1 kHz. A glass sample with thickness of 1.5 mm was installed on a motorized translation stage, and translated along the beam axis with respect to focal plane on the distance of 120 mm.

All samples exhibit positive nonlinearity. The dependences of nonlinear coefficient γ on the energy in femtosecond pulse for tungstate- tellurite glasses are presented on Figure 1. The maximal γ values were obtained for bismuth oxide modified glasses: $\gamma = 5.6 \cdot 10^{-6}$ cm^2/GW, lowest nonlinear coefficients among glasses investigated were obtained for zinc-tellurite glasses ($\gamma \approx 10^{-6}$ cm^2/GW).

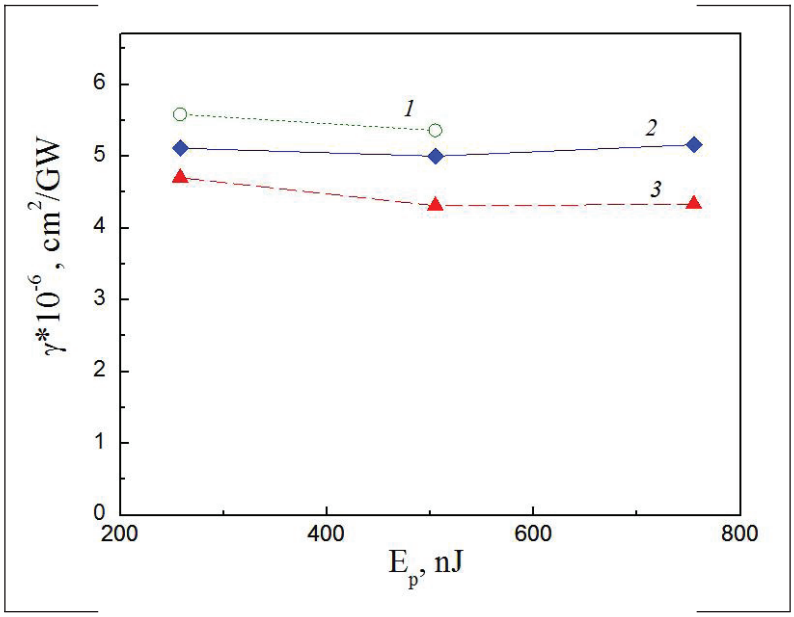

Figure 1. The dependences of Kerr nonlinearity coefficient γ on pulse energy for various tungstate-tellurite glasses: *1* - bismuth oxide modified glasses; *2* – molybdenum and lanthanum oxides modified glasses; and *3* - lanthanum oxide modified glasses.

Tungstate-tellurite glasses modified with bismuth, molybdenum or lanthanum oxides were tested for femtosecond direct writing of waveguide tracks. To this end, fs-laser beam was focused in the bulk of glass plate with objective of numerical aperture NA=0.85 and series of tracks were inscribed under wide range of pulse energies, repetition rates, and scan speeds.

All obtained tracks exhibit decreased refractive index with respect to non-modified region of sample. The highest value of refractive index change was about *Dn* = - 0.002 produced in molybdenum and lanthanum oxides modified tungstate-tellurite glass. The series of tracks in this sample recorded for different pulse energies is shown in Figure 2. Threshold energy required for glass modification was E_{tr} = 14 nJ. The tracks were smooth and homogeneous at wide energy range *E* = 14 ÷ 160 nJ.

The results of the study evidence high potential of tellurite oxide based glasses for realization of nonlinear waveguide devices.

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M.P. Smayev, V.V. Dorofeev, A.G. Okhrimchuk

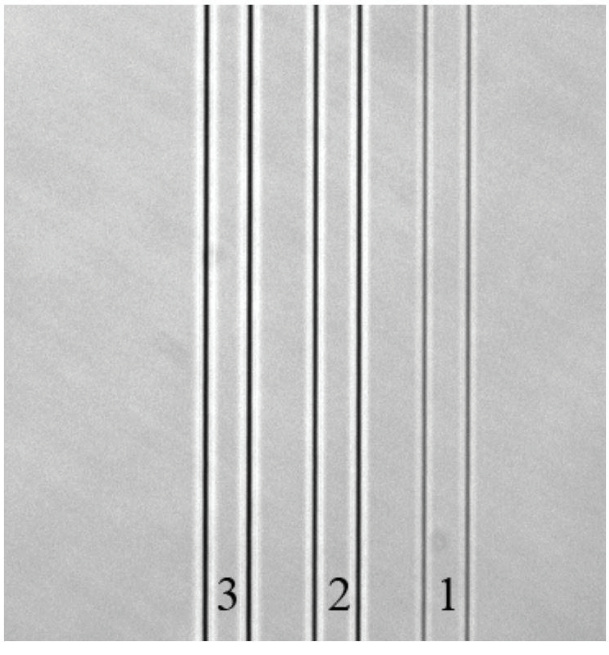

Figure 2. The series of tracks with modified refractive index inscribed in molybdenum and lanthanum oxides modified tungstate-tellurite glass by femtosecond pulses with different energies: *1* – E_p = 30 nJ; *2* – E_p = 60 nJ; *3* – E_p = 90 nJ.

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SCIENTIFIC ORGANIZATION

Immanuel Kant Baltic Federal University

Development of X-ray refractive optics. New promising prospectives for diffraction limited 4-th generation X-ray sources

ABSTRACT

After the first successful experimental demonstration 20 years ago, the use of X-ray refractive optics has rapidly expanded and they are now in common use at 15 synchrotrons in 10 countries. This development has intensified after the successful implementation of transfocators - tunable devices based on refractive lenses. In addition to traditional micro-focusing applications, the transfocators can provide the following beam conditioning functions: condensers with a tunable beam size, micro-radian collimators, low-band pass filters and high harmonics rejecters.

KEYWORDS

Synchrotron radiation, X-ray optics, refractive lenses, microscopy, interferometry, imaging.

ACKNOWLEDGEMENTS

The results of the project were achieved with support of the Ministry of Education and Science of the Russian Federation as a part of the agreement № 14.Y26.31.0002 under the program to attract scientists in the Russia with a worldwide reputation for creating a competitive research laboratories launched by the Russian Federation Government Decree № 220.

SUMMARY

After the first successful experimental demonstration 20 years ago [1], the use of X-ray refractive optics has rapidly expanded and they are now in common use at 15 synchrotrons in 10 countries. This development has intensified after the successful implementation of transfocators - tunable devices based on refractive lenses [2]. In addition to traditional micro-focusing applications, the transfocators can provide the following beam conditioning functions in the energy range from 3 to 100 (200) keV:

- condensers with a tunable beam size,
- micro-radian collimators ,
- low-band pass filters - monochromator [2]
- high harmonics rejecters [3]

New advanced parameters of the beam provided by the diffraction limited sources – XFELs and new synchrotrons with the reduced horizontal emittance will open up a unique opportunity to build up a new concept for the loss-free beam transport and conditioning systems based on in-line refractive optics. Taking an advantage of the substantially reduced horizontal source size and the beam divergence these new systems integrated into the front-end can transfer the photon beam almost without losses from the front-end to any further secondary optical systems (mirrors, crystals, lenses etc.) or directly to the end-stations. Evidently, beamlines will benefit from the possibility to include active moveable lens systems in the front-ends. In this regard, development of diamond refractive optics is crucial [4,5]. The implementation of the lens-based beam transport concept will significantly simplify the layout of majority of the new beamlines [6]. It will also allow a smooth beamlines transition from the present beam parameters to the upgraded ones, avoiding major optics modifications [7].

The field of applications of refractive optics is not limited to beam conditioning, but can be extended into the area of Fourier optics, as well as coherent diffraction and imaging techniques [8-13]. Using the intrinsic property of the refractive lens as a Fourier transformer, the coherent diffraction microscopy and high resolution diffraction methods have been proposed to study 3-D structures of semiconductor crystals and mesoscopic materials [14–15].

Another promising direction of refractive optics development is in-line X-ray interferometry. Recently proposed bi- and multi-lens interferometers can generate an interference field with a variable period ranging from tens of nanometers to tens of micrometers [15,16]. This simple way to create an X-ray standing wave in paraxial geometry opens up the opportunity to develop new X-ray interferometry techniques to study natural and advanced man-made nano-scale materials, such as self-organized bio-systems, photonic and colloidal crystals, and nano-electronics materials. As a classical interferometer it can be used for phase contrast imaging and radiography. Finally it can be useful for the coherence characterization of the X-rays sources and free electron lasers.

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ADDITIONAL INFORMATION

Obtained Russian patents under the agreement № 14.Y26.31.0002: 1. Obtained Russian patent Reg. Number 155377 from 09.09.2015 «A device for determining optical characteristics according to the interference pattern» Authors: P.Ershov, N. Klimova, I Lyatun, M Polikarpov, Applicant: FGAOU VO “BFU Immanuel Kant.” Àpplication Reg. Number 2014147857 from 27.11.2014. 2. Obtained Russian patent Reg. Number « A device for determining the optical properties of materials on the basis of anomalous refraction in refractive optical elements» Authors: P.Ershov, N. Klimova, I Lyatun, M Polikarpov, Applicant: FGAOU VO “BFU Immanuel Kant.” Àpplication Reg. Number 2014147855 from 27.11.2014. The decision to grant a patent from 12.15.2015. Àpplications for the grant of a Russian patent under the agreement № 14.Y26.31.0002: : 1. Àpplication for the grant of a Russian patent « X-ray tube with a composite anode » Authors: A.Goikhman, N. Klimova, S. Savelyev, Applicant: FGAOU VO “BFU Immanuel Kant.” Reg. Number 2015150259 from 24.11.2015. The continued examination of the merits. 2. Àpplication for the grant of a Russian patent «Automated slit device» Authors: A.Goikhman, N. Klimova, P. Prokopovich, I.Panormov, Applicant: FGAOU VO “BFU Immanuel Kant.” Reg. Number 2015150260 from 24.11.2015. The continued examination of the merits. 3. Àpplication for the grant of a Russian patent «Test bench for refractive X-ray optics» Authors: A.Goikhman, P. Prokopovich, A. Borisov, I.Panormov, N. Klimova, P.Ershov, D.Serebrennikov, D.Zverev, A.Barannikov, Applicant: FGAOU VO “BFU Immanuel Kant.” Reg. Number 2015155999 from 12.25.2015. The continued examination of the merits.

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Coherent hard X-ray microscopy for the characterization of mesoscopic materials

SCIENTIFIC ORGANIZATION

European Synchrotron Radiation Facility

ABSTRACT

We present a coherent high energy X-ray microscope to study the wide range of natural and artificial mesoscopic materials that are structured on scales of the order of a few microns to a few hundred nanometers. The concept of the proposed microscope is based on employing compound refractive lenses allowing to retrieve high resolution diffraction pattern and real-space images in the same experimental setup. This idea, well-known for the studies of crystals by high resolution transmission electron microscopy, is the key ingredient of our approach.

KEYWORDS

X-ray optics, refractive lenses, microscopy.

ACKNOWLEDGEMENTS

The work was supported by the Ministry of Science and Education of Russian Federation grants № 14.Y26.31.0002.

SUMMARY

We present a coherent high energy X-ray microscope to study the wide range of natural and artificial mesoscopic materials that are structured on scales of the order of a few to a a few hundred nanometers. The concept of the proposed microscope is based on employing compound refractive lenses allowing to retrieve high resolution diffraction pattern and real-space images in the same experimental setup [1-4]. This idea, well-known for the studies of crystals by high resolution transmission electron microscopy, is the key ingredient of our approach.

The microscope operates under a coherent illumination where a diffraction pattern of the specimen is formed in the back focal plane of the condenser and an inverted two-dimensional image of the object is formed by objective lens in the image plane [5]. The diffraction mode is used to investigate the structure over the macroscopic distances and to orient the crystals parallel to the low index direction to perform high-resolution imaging on the local scale. The image formation relies on phase contrast due to the interference of several diffracted beams [6]. A high spatial coherence is needed in the imaging mode to ensure a reasonable contrast. The coherence in terms of the angular source size determines the lens angular resolution (< 1microrad) to get high resolution diffraction patterns.

Functioning at 10 – 30 keV, the microscope is one of the brunches of the multimodal instrument which is under the development at the ID06 ESRF beamline. It consists of the condenser, the objective lens and two X-ray CCD cameras – large area detector for diffraction and high resolution CCD for imaging. Condenser and objective assemblies are comprised of Be parabolic refractive lenses. Switching from the diffraction mode to the imaging is achieved by placing the objective lens into the beam, and the chosen detector. The tunable objective lens offers full-field imaging with variable resolution and field of view. It allows for the identification of features of interest in a coarse resolution overview before increasing magnification to study these features with maximum resolution. At present, at the maximum magnification a resolution of 100 nm is achieved, but it should be noted that the studies on its improvement are curred out and in the near future we can expect resolution about 30 nm.

The microscope was applied for study of natural and synthetic opals, metal inverted photonic crystals and colloidal suspensions [5,7]. The combination of the direct-space imaging and high resolution diffraction provide a wealth of information on their local structure and the long range periodic order. The concept of the hard x-ray microscope emerged concomitantly with the realization that the ESRF source upgrade would, through the greatly enhanced brilliance and fraction of coherent light, open entirely new frontiers in materials imaging [8]. Short acquisition times with modern area detectors allow to extend the microscope to time-resolved

studies of the crystallization dynamics, response of the mesoscopic structures to external stimuli such as mechanical strain, temperature jump or temperature gradient as well as external fields.

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ADDITIONAL INFORMATION

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Leading researcher

New hybrid MOF-based nanomaterials for storage and delivery of bioactive compounds

SCIENTIFIC ORGANIZATION

Southern Federal University

ABSTRACT

Hybrid MOF-based nanomaterials for storage and delivery of bioactive compounds have been synthesized. The periodic structure have been studied by means of X-ray diffraction. Local atomic and electronic structure have been studied by means of element specific X-ray Absorption Spectroscopy. FTIR-spectroscopy has been used to monitor the adsorption of guest molecules inside pores.

KEYWORDS

Hybrid nanomaterials, bioactive materials, Metal-organic frameworks.

ACKNOWLEDGEMENTS

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SUMMARY

One of the major problem in biomedicine technologies is nontoxic nanomaterials for drug storage and delivery. The limiting characteristics of existing materials are low efficiency loading (about 5 mass percent) and fast drug realize. Porous MOF-based hybrid nanomaterials have a possibility of fine tuning of structure and properties. The later is a result of a wide variety of organic linkers and metal clusters that compose the framework structure. Biomedical applications of metal-organic frameworks is a novel trend that develops at a record breaking pace. The later resulting in the number of original research papers[1-6] and fundamental reviews[7-9].

Such hybrid MOF-based nanomaterials for storage and delivery of bioactive compounds have been synthesized. The periodic structure have been studied by means

of X-ray diffraction. Local atomic and electronic structure have been studied by means of element specific X-ray Absorption Spectroscopy. FTIR-spectroscopy has been used to monitor the adsorption of guest molecules inside pores. Biological activity have been studied in non pathogenic bacteria.

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Morphology transition mechanism from icosahedral to decahedral phase during growth of nanoclusters

SCIENTIFIC ORGANIZATION

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ABSTRACT

The morphology transition from the thermodynamically favorable to the unfavorable phase during growth of free-standing copper nanoclusters is studied by molecular dynamics simulations. A universal mechanism of a solid-solid transition, from icosahedral to decahedral morphology in nanoclusters, is proposed. We show that a formation of distorted NC during the growth process with islands of incoming atoms localized in certain parts of the grown particle may shift the energy balance between Ih and Dh phases in favour of the latter.

KEYWORDS

Nanoclusters, morphology transition, molecular dynamics, nanoclusters growth.

SUMMARY

The study of metal nanoclusters has been a subject of intense research activities in recent years. This is due to their great importance in variety of applications. Besides, such objects are intermediate between single atoms and molecules and bulk matter, and their properties may qualitatively differ. Properties of nanocluster crucially depend on growth methods and conditions during the process. Understanding of the growth process at the early stages is of particular interest since the morphology of the seed may determine structure of big clusters.

The morphology transition from the thermodynamically favorable to the unfavorable phase during growth of free-standing copper nanoclusters is studied by molecular dynamics simulations. We give a detailed description of the kinetics and thermodynamics of the process. A universal mechanism of a solid-solid transition, from icosahedral to decahedral morphology in nanoclusters, is proposed. We show that a formation of distorted NC during the growth process with islands of incoming atoms localized in certain parts of the grown particle may shift the energy balance between Ih and Dh phases in favour of the latter leading to the morphology transition deep within the thermodynamic stability field of the former. The role of diffusion in the morphology transition is revealed. In particular, it is shown that fast diffusion should suppress the morphology transition and favour homogeneous growth of the nanoclusters.

Tignon Jerome
Dr.
Professor

TeraHertz

SCIENTIFIC ORGANIZATION

Ecole Normale Superieure / UPMC

ABSTRACT

The Tera-Hertz (THz) frequency range, in the far-infrared domain of the electromagnetic spectrum, is also known as the “THz gap”. With respect to its optics or electronics neighbors, the development of sources or detectors is more difficult in this region of the spectrum. These “T-rays” are nonetheless at the basis of very interesting applications for spectroscopy, security-imaging, non-destructive control, explosive detection, etc. The talk will review these properties as well as modern technics such as THz time-domain spectroscopy.

KEYWORDS

TeraHertz, spectroscopy, ultrafast.

SUMMARY

T-rays spectroscopy

respect to its optics or electronics neighbors, the development of sources or detectors is more difficult in this region of the spectrum. These “T-rays” are nonetheless at the basis of very interesting applications for spectroscopy, security-imaging, non-destructive control, explosive detection, etc. The talk will review these properties as well as modern technics such as THz time-domain spectroscopy.

Tikhonov Evgeny
Postgraduate student
Junior researcher

Andreev reflection and shot noise in a diffusive 3D topological insulator proximized by a superconductor

SCIENTIFIC ORGANIZATION

Moscow Institute of Physics and Technology

ABSTRACT

We experimentally study transport and shot noise in lateral N-TI-N and N-TI-S contacts defined on thin flakes of three-dimensional topological insulator Bi1.5Sb0.5Te1.7Se1.3 (N - normal metal, S - s-type superconductor). Via shot noise measurements we demonstrate the elastic diffusive transport regime in both N-TI-S contacts, subjected to the perpendicular magnetic field, and in N-TI-N contacts. In zero magnetic field, we show the Andreev reflection regime in N-TI-S contacts. Our measurements allow to extract the value of a proximity induced gap in the range ~0.3meV.

KEYWORDS

Topological insulator, superconductivity, andreev reflection.

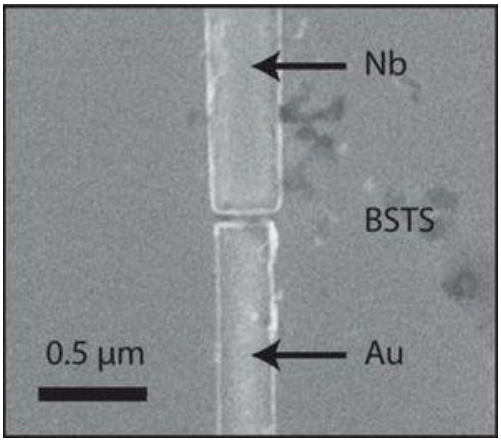
ACKNOWLEDGEMENTS

We thank Y.Huang and M.S.Golden for the crystal growth. This work was supported by the Russian Academy of Sciences, the Ministry of Education and Science of the Russian Federation Grant No.14Y.26.31.0007, the RFBR Grants 16-32-00869 and 15-02-04285 and the Russian Science Foundation project no. 15-12-30030.

SUMMARY

1) Intro;

2) Sample layout:

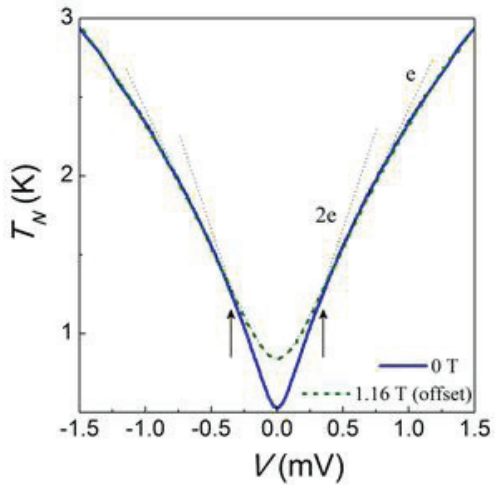


3) Magnetotransport data;

4) Shot noise and transport in the N-TI-N device: diffusive transport evidenced by the universal value of the Fano-factor $F_{\mathrm{N}} \approx 1/3$;

5) Shot noise and transport in N-TI-S devices: effective charge doubling and the Fano-factor $F_{\mathrm{AR}} \approx 0.22 \pm 0.02$ in zero magnetic field; diffusive transport and the Fano-factor $F_{\mathrm{N}} \approx 1/3$ in magnetic field;

6) Finite bias 2e⟶e transition and proximity gap extraction



ADDITIONAL INFORMATION

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Four-wave mixing effect in quantum beats and Rabi oscillations in semiconductor heterostructures

SCIENTIFIC ORGANIZATION

Saint Petersburg State University

ABSTRACT

Quantum beats of quantum-confined exciton states in quantum wells and Rabi oscillations in heterostructures with microcavities are experimentally studied by pump-probe method. Analysis of experimental data has shown certain similarity in the physical mechanism of oscillating signals in spite of fundamental difference of the systems. It will be shown in the presentation that the oscillations are caused by the interference of the four-wave mixing signal with the polarization created in the exciton or polariton system by the probe beam.

KEYWORDS

Quantum wells, microcavities, quantum beats, nanoheterostructures.

ACKNOWLEDGEMENTS

11.G34.31.0067

SUMMARY

The experimental manifestation of coherence of optical excitations in these systems. Study of coherent phenomena is important from both the fundamental and practical points of view because the optical coherence may be used for realization of quantum computing. One of the most effective methods of the coherence detection is the two-pulse pump-probe method when the first (pump) pulse creates a coherent state of the system and the second (probe) one delayed in time detects evolution of the state. This method is typically used in one of the two possible geometries of experiment. The first one is the pump-probe geometry when the signal is detected in the direction of the transmitted or reflected probe beam. The second one is the four-wave mixing geometry when the signal is detected in the direction of the pump beam diffracted at the grating created in the structure by joint action of the mump and probe beams. It is important that the four-wave mixing signal persists while the optical coherence is conserved. At the same time, for the quantum beat signal, the mutual coherence of excited states is only required. So, a comparative study of these two signals allows one to identify the nature of coherence in the structure. In this work, we demonstrate that such comparative study can be performed in one geometry of experiment.

We have used ordinary pump-probe geometry. An integral intensity of the transmitted or reflected probe beam is detected as a function of the delay between the pump and probe pulses. A femtosecond Ti:sapphire laser with the pulse repetition rate of 80 MHz is used. Quantum beats of the quantum confined excitons states are studied in sample A with a 95-nm InGaAs/GaAs quantum well with the 3% of indium content. Rabi oscillations are observed in sample B with a microcavity containing four 10-nm InGaAs/GaAs quantum wells with 6% of indium sandwiched between two Bragg reflectors. The laser spots on the samples are of about 50 mkm. The sample temperature is of 4 K.

The experiments have shown clearly observable oscillations of the pump-probe signal for both the samples as for positive as for negative delay of the probe pulses relative to the pump ones. Analysis shows [1] that the oscillating signal detected at the negative delays is due to the four-wave mixing effect detected at the non-standard direction. The beat frequencies observed for sample A correspond to the energy distances between quantum-confined exciton states and, therefore, are attributed to the quantum beats of these states. For sample B, the observed beat frequency corresponds to the splitting of the upper and lower polariton states and is attributed to the vacuum Rabi oscillations. Comparison of the oscillation signal decays for the positive and negative delays gives rise to valuable information about the decoherence processes in the structures under study.

[1] Trifonov, A. V., Gerlovin, I. Y., Ignatiev, I. V., Yugova, I. A., Cherbunin, R. V., Efimov, Y. P., ... & Kavokin, A. V. (2015). Multiple-frequency quantum beats of quantum confined exciton states. *Physical Review B*, *92*(20), 201301.

Ueda Keniti
Doctor of Science
Professor Emeritus

Development of the laboratory of the diagnostics of novel optical materials for advanced lasers in 2013 – 2015

SCIENTIFIC ORGANIZATION

University of Electro-Communications

ABSTRACT

The “Laboratory for Diagnostics of New Optical Materials for Advanced Lasers” to perform high-level world-class research and solve topical problems of creating lasers with high peak and average power aiming at improving their consumer properties was established. The results of the carried out research were published in more than 34 papers in high-rate peer-reviewed journals, presented at about 100 different Russian and international conferences. 14 applications were submitted for recording the intellectual property rights.

KEYWORDS

High power lasers, optical media properties, laser ceramics, cryogenic cooling.

ACKNOWLEDGEMENTS

This work was supported by the mega-grant of the Government of the Russian Federation No. 14.B25.31.0024 executed at the Institute of Applied Physics of the Russian Academy of Sciences.

SUMMARY

Introduction

In the last years a large number of promising laser media has appeared. It is connected with rapid developing the technology of producing the laser and optical ceramics, which allows to obtain active and optical elements faster, cheaper, larger, with a higher concentration and homogeneity of the active ion; to obtain the ceramics from a variety of materials, including the materials which are technologically impossible to grow in a single crystal form. The comprehensive investigation of media properties (laser, thermo-optic, nonlinear optical, spectral, etc.) is relevant for laser systems for efficiency improvement, new types of lasers creation and spread its use in scientific experiments as well as for practical purposes. The measurement of material constants and its dependences on temperature, wavelength, the concentration of the active ion etc. for new promising laser materials allows its properties optimizing and obtaining the unique characteristics of the optical elements for advanced lasers.

Goals and objectives of the scientific research project activities

The principal goal of the project was establishing the “Laboratory for Diagnostics of New Optical Materials for Advanced Lasers”, that would allow performing high-level world-class research and solve topical problems of creating lasers with high peak and average power aiming at improving their consumer properties.

The main tasks of the project were production and diagnostics of new optical materials (ceramics, crystals, and glasses) and development on their basis of optical units (laser components) with unique characteristics. The diagnostics included development of measurement benches, measurement techniques, and software for measuring different characteristics (photoelastic, thermo-optical, laser, magneto-optical, spectral) of the new materials. At the stage of developing optical units (quantum amplifiers, optical isolators), with the aim to improve their characteristics it was intended to study the opportunities for reducing and compensating parasitic effects. It was also planned to improve the methods of creating new media (sintering of ceramics, crystal growth). The implementation of the project was supposed to advance a number of critical/concurrent technologies (creating composite elements, effective heat sinks, sources of constant magnetic fields, etc.).

Scientific research project activities

In the course of project implementation, methods for measuring photoelastic, thermo-optical, nonlinear-optical, laser, magneto-optical and spectral characteristics in the 80…300K temperature range were developed for optical media diagnostics. 12 measurement benches with the corresponding software for processing experimental data were created.

1. Photoelastic constant meter.
2. Meter of Verdet constant and magneto-optical figure of merit in the 80…300 K temperature range.
3. 2D-scanning Hartman sensor.
4. Meter of nonlinear optical susceptibility.
5. Meter of mechanical resistance of coatings, surface and bulk damage threshold.
6. Meter of thermal resistance of solid body contacts.
7. Meter of thermal conductivity of solids.
8. Meter of laser media characteristics.
9. Profilometer.
10. Measurer of spectral characteristics.
11. Measurer of thermo-optical characteristics.
12. Gage of the temperature dependence of thermo-optical constants.

The developed techniques and measurement benches were used to conduct theoretical and experimental studies of the following characteristics of different optical media:

- optical (refractive index inhomogeneity, depolarization ratio, and others);

- thermo-optical (thermal conductance, thermal expansion coefficient, and others);

- magneto-optical (Verdet constant, magneto-optical figure of merit).

The impact of variations of these characteristics on optical beam propagation was investigated.

Methods of producing new laser media: ceramic (techniques of synthesizing nano-powders with characteristics demanded for laser ceramics, of compacting ceramics with high homogeneity, and of high-temperature sintering of TAG and YAG ceramics), and monocrystalline (development of an optimal method of growing garnet, terbium phianite and terbium vanadate crystals, quality studies of TSAG crystals of different compositions) were developed and upgraded.

Theoretical and experimental studies of weak signal gain (stored energy) and total gain (multipass, using a regenerative amplifier, and so on), cw generation modes, Q-switching, nonlinear optical conversion of radiation, reduction of parasitic thermal effects etc. were carried out for different laser components.

An important part of the work was creation of two technological benches:

- for thermodiffusion bonding of optical elements, and

- for producing sources of magnetic fields.

Results

Based on the results of the research and the works performed on the 12 created measurement and 2 technological benches, the following devices were developed:

- cryogenic Yb:YAG disk laser (MOPA circuit; energy 54 mJ at a pulse repetition rate of 200 Hz and pump energy of 200 mJ; energy 30 mJ at a pulse repetition rate of 1 kHz and cw pumping);

- disk laser head (comprising high-efficiency AE water cooling system and optical multipass pump input scheme; weak signal gain of 1.25 at a stored energy of 400 mJ was attained);

- cryogenic disk laser head (AE aperture of 20 mm);

- polarization apodizing diaphragm (allows correcting e.m. radiation distribution in the optical range);

- Faraday isolator on a shortened element (30 dB at a power of 650 W);

- Faraday isolators on a new medium – TAG and Ce:TAG ceramics;

- Faraday isolators on TGG ceramics (with internal compensation: 30 dB up to 2.7 kW; with external compensation: 30 dB up to 2 kW; traditional scheme: 30 dB up to 1 kW; cryogenic: 30 dB over 2 kW);

- Faraday isolator with magnetic system having preset field inhomogeneity (7-fold reduction of depolarization level);

- Faraday isolator on a new medium – TSAG crystal;

- large-aperture Faraday isolator (on a TGG crystal having aperture of 30 mm (33.5 dB at 1.5 kW).

Also, the following crystal samples were manufactured: TSAG, Tb-containing phianite, terbium vanadate, and optical ceramics: TAG, YAG, $MgAl_2O_4$ doped by a Tm^{3+} ion.

Conclusion

The developed material base (measurement and technological benches) and the professional skill of the team allow obtaining world level results. Based on the results of the carried out research we developed and manufactured prototypes of optical units with unique characteristics, including laser oscillators, amplifiers, Faraday isolators with water and cryogenic cooling having different configurations of active and magnetooptical elements and heat sinks. Using the developed technologies we manufactured samples of TSAG, Tb-containing phianite and terbium vanadate crystals and samples of optical ceramics: TAG, YAG, and Tm^{3+} ion activated $MgAl_2O_4$.

The results of the carried out research were published in more than 34 papers in high-rate peer-reviewed journals, presented at about 100 different Russian and international conferences. 14 applications were submitted for recording the intellectual property rights. These indicators confirm the high scientific and technical level of the research results that correspond to or excel the best world's achievements in the field of optical media diagnostics, creation of composite optical elements, manufacturing magnetic systems with record values of magnetic field intensity, optical units and components with unique characteristics.

Ustinov Alexey
Professor
Head of the laboratory

Superconducting metamaterials

SCIENTIFIC ORGANIZATION

National University of Science and Technology MISIS

ABSTRACT

Metamaterials are artificial engineered media that enable tailored interactions with electromagnetic waves. The design flexibility of superconducting thin-film resonators and Josephson circuits allows for utilizing small structures down to the nanoscale while maintaining low loss properties, very strong and well-controlled nonlinearity, and frequency tunability in the microwave and mm-wave frequency ranges. An interesting spin-off here is going to be quantum metamaterials comprised of arrays of superconducting qubits.

KEYWORDS

Superconductivity, metamaterials, Josephson junctions, qubits.

ACKNOWLEDGEMENTS

Partial support by the Ministry of Education and Science of Russian Federation in the framework of Increase Competitiveness Program of the NUST MISIS (contracts no. K2-2014-025 and K2-2015-002) is gratefully acknowledged.

SUMMARY

I will review progress in the development of superconducting metamaterials. There are several distinct advantages and unique properties brought to the metamaterials field by superconductivity. These include the low-loss nature of the meta-atoms, their compact structure, their extraordinary degree of nonlinearity and tunability, magnetic flux quantization and the Josephson effect, quantum effects in which photons interact with quantized energy levels in the meta-atom, as well as strong diamagnetism.

Vlasenko Leonid
Doctor of Science
Principal scientist

Spin dependent phenomena and magnetic resonance studies of point defects in silicon and silicon structures

SCIENTIFIC ORGANIZATION

Ioffe Institute of Russian Academy of Science

ABSTRACT

Highly sensitive methods for detection magnetic resonance based on spin dependent microwave photoconductivity were developed and applied for investigation the microscopic structure of the recombination centers and their excited states in silicon and silicon structures. The main attention is given to study the new paramagnetic centers observed in silicon, silicon p-n junctions and silicon/silicon dioxide structures and created by irradiation, ion implantation, high temperature annealing, oxidization and chemical treatments usually used in semiconductor technology.

KEYWORDS

Semiconductors, magnetic resonance, spin dependent phenomena, silicon, recombination centers.

ACKNOWLEDGEMENTS

This work was supported by the Megagrant of the Russian Government, project 14.Z50.31.0021.

SUMMARY

1. In general, spin dependent recombination (SDR) is the well known physical phenomenon when the recombination rate of non-equilibrium electrons and holes in semiconductors excited by light or injected in p-n junctions depends on the relative spin orientations of carriers and recombination centers. Spin orientation can be changed by excitation of electron paramagnetic resonance (EPR) increasing the recombination rate and, consequently, decreasing the conductivity of samples. The most of experiments on EDMR were performed using standard EPR spectrometers for excitation of magnetic resonance whereas the EPR signals were detected monitoring dc-current through the sample. In the present work the contact free method was used for detection of SDR-EPR spectra of recombination centers. This method is based on the absorption of the electrical component of microwave field by free carriers whereas the magnetic component in microwave cavity is used for magnetic resonance excitation.

2. It was shown that the detection EPR spectra of recombination centers in silicon using the spin dependent microwave photoconductivity has four orders higher sensitivity compare to the traditional EPR spectroscopy. The developed methods can be applied for monitoring, diagnostic and investigations of different defects at their low concentration created by fabrication processes and during the operation of semiconductor devices.

3. Physical mechanisms of spin dependent recombination of photo excited (or injected in p-n junctions) carriers via the excited triplet (spin S=1) states of recombination centers were investigated and new SDR detected spin S=1 EPR spectra were found. Particularly, new SDR-EPR spectra of low symmetry modifications of well known complexes of oxygen-vacancy (O+V) and carbon related centers in silicon were observed under annealing of irradiated silicon in the temperature range of 350 - 500 ^{O}C. The models of low symmetry configurations of the considered centers were suggested.

4. The excited triplet states of recombination centers are metastable and have relative long life time, up to milliseconds, and form the energy levels in silicon band gap. Analyzing the temperature dependences of SDR-EPR spectra The energy level positions of E_C - 0.095 eV and E_C – 0.25 eV were estimated for the excited triplet states of the O+V and carbon related centers, respectively.

5. The processes of spin SDR included the creation of the excited triplet states of recombination centers were considered in the space-charge layer of silicon p-n junctions. The SDR-EPR spectra were detected monitoring the forward current through p-n junctions without illumination. It was shown that paramagnetic recombination centers and their excited triplet states can be detected even without

excitation of magnetic resonance when sharp lines of the conductivity changes are observed at the points of magnetic field corresponding to the anticrossing of magnetic sublevels or to the coincidences of Zeeman frequencies of different paramagnetic recombination centers.

6. SDR effects were applied for study the surface recombination centers in commercially produced silicon wafers. It was found that such centers are always observed even without any additional treatments of surface. New centers on (100) oriented wafers were found and investigated. Analysis of their SDR-EPR spectra allows us to suggest the model of new centers as the closed pairs of dangling Si bonds in Si/SiO_2 layer. It was found that such parameters of new spectra as a line width, line positions, fine and hyperfine structure splittings depend on the thickness of SiO_2 layer. These parameters are changed gradually during 10-12 days after removal SiO_2 by chemical etching in fluoride acid and following slow surface oxidization on air at room temperature.

Zakharov Vladimir

Doctor of Sciences, full member of the RAS

Head of Laboratory; Regents' Professor

SCIENTIFIC ORGANIZATION

Novosibirsk State University; University of Arizona

Weak-turbulent theory of wind-driven sea

ABSTRACT

We developed the weak-turbulent theory of wind-driven sea using regular methods of theoretical physics. The key point that made it possible is existence of natural dimensionless small parameter: the ratio of air and water density. As far as this parameter is really small, about 1/1000, the main physical process on the sea surface is the nonlinear interaction of weakly nonlinear waves. This process allows the self-consistent statistical description which can be performed in terms of kinetic equation for wave spectra, similar to kinetic equation used in the solid state physics.

KEYWORDS

Weak-turbulent theory, nonlinear waves.

ACKNOWLEDGEMENTS

The author thanks for the support of the Russian Science Foundation (Grand No. 14-22-00174).

SUMMARY

We developed the weak-turbulent theory of wind-driven sea using regular methods of theoretical physics. The key point that made it possible is existence of natural dimensionless small parameter: the ratio of air and water density. As far as this parameter is really small, about 1/1000, the main physical process on the sea surface is the nonlinear interaction of weakly nonlinear waves. This process allows the self-consistent statistical description which can be performed in terms of kinetic equation for wave spectra, similar to kinetic equation used in the solid state physics. The kinetic equation derived “from first principle” has a rich family of exact solutions both stationary and self-similar. Free parameters in these solutions can be chosen by taking into account the interaction with turbulent atmospheric boundary layer. Interaction with wind can be described by few empirical parameters found by comparison of numerical solution of kinetic equation with experimental data on wave spectra in open sea and in laboratory. The developed theory of wind-driven sea describes perfectly the shape of spectra and their dependence on space and time. This theory can be used as a base for well-justified models for wave forecasting.

Zapasskii Valerii
Doctor of Sciences
Leading Researcher

Optics of spin noise in semiconductors

SCIENTIFIC ORGANIZATION

Spin Optics Laboratory, St.-Petersburg State University

ABSTRACT

The spin noise spectroscopy represents, at present, a new, highly efficient method of research with unique and somewhat curious properties. Generally, it does not imply any perturbation of the system and, at the same time, may exhibit properties more typical for nonlinear optics. During the last several years, many new opportunities provided by the spin-noise technique have been discovered and used for studying spin-system dynamics in semiconductors. Recent results show that the spectroscopy of spin noise is a promising method of research with still underestimated potential.

KEYWORDS

Spin noise spectroscopy, spin dynamics, magnetic resonance, magneto-optics.

ACKNOWLEDGEMENTS

The RFBR and DFG in the frame of International Collaborative Research Center TRR 160 (project No.~15-52-12013) are acknowledged.

Zverev Dmitrii
Master's Degrees
Engineer

High-Resolution X-ray Diffraction Based on Refractive Lenses

SCIENTIFIC ORGANIZATION

Immanuel Kant Baltic Federal University

ABSTRACT

To demonstrate the possibilities of the proposed high-resolution X-ray diffractometry using Fourier optics, experiments using coherent synchrotron radiation source were performed. By means of this method a specially prepared diffractive microstructure were examined. In addition, we investigated the Si-Ge nano-heterostructures that are 100 nm germanium nano-crystals, standing on a periodic grid of the silicon pillars. The obtained results allowed to get detailed information on the periodicity, spatial orientation and crystalline perfection of the structures under study.

KEYWORDS

X-ray compound refractive lens, Fourier optics, Bragg reflection, X-ray diffraction, microstructure, heterostructure, nano-crystal, nanostructure.

SUMMARY

One of the promising areas of nano- and microelectronics is the development of technologies for the production of 3D small sized semiconductor structures. One example is the detection of electromagnetic radiation by complementary metal oxide semiconductor (CMOS) matrices where millions of pixels (semiconductor heterostructures) are arranged on the substrate. Creating a new, more complex structures with unique properties, as well as the development of production technology, in turn, implies the improvement of methods of their study. The paper presents a method for studying such structures, which allows to exceed the resolution of the classical method of X-ray diffraction.

The method is based on the idea of using X-ray refractive lenses as a Fourier transformer. Thus, the X-ray CCD camera is placed in the image plane of the lens, and the lens itself can be placed before or after the structures under study. In this geometry, the refractive lens acts as a high-resolution analyzer of the wavefront, which is formed as a result of X-ray diffraction on the ordered crystal structures

in Bragg geometry. The advantages of the proposed method are as follows: the flexibility of experimental setup; convenience of adjustment and measurement as compared to the classical methods of X-ray diffraction; the possibility of reducing the duration of the experiments; high angular resolution; and the ability to observe the reflection from the crystal in a certain range of incidence angles.

To demonstrate the possibilities of the proposed high-resolution X-ray diffractometry using Fourier optics, experiments using coherent synchrotron radiation source were performed. By means of this method a specially prepared diffractive microstructure were examined. These structures were manufactured on the single-crystal silicon wafer using precision ion beamlithography. In addition, we investigated the Si-Ge nano-heterostructures that are 100 nanometer germanium nano-crystals, standing on a periodic grid of the silicon pillars, with width of 90 nanometers and a height of 150 nanometers. The obtained results allowed to get detailed information on the periodicity, spatial orientation and crystalline perfection of the structures under study.

ADDITIONAL INFORMATION

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