Latvija 100

INSTITUTE OF SOLID STATE PHYSICS
UNIVERSITY OF LATVIA

1978
2018

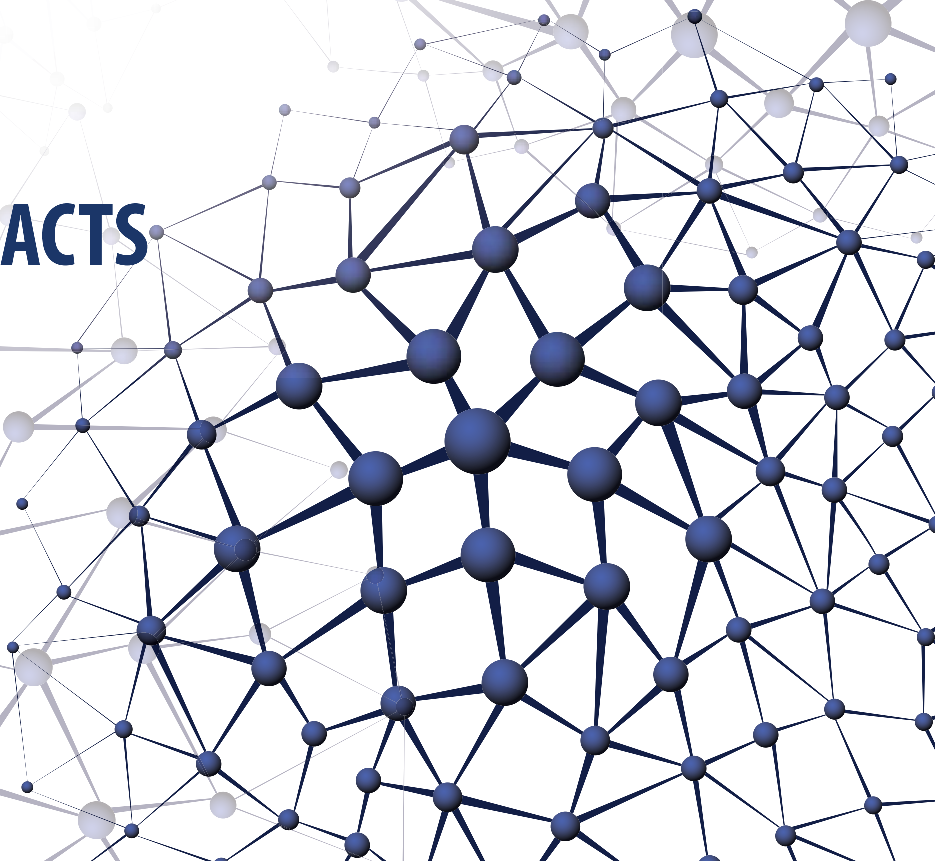
FUNCTIONAL MATERIALS
& NANOTECHNOLOGIES

12th International Scientific Conference on Functional Materials and Nanotechnologies

FM&NT-2018

October 2- 5, 2018,
Riga, Latvia

BOOK OF ABSTRACTS



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Riga, 2018

WELCOME MESSAGE TO
FM&NT-2018 PARTICIPANTS

DEAR COLLEAGUES,

It is my great pleasure to welcome you at the 12th International Conference Functional Materials and Nanotechnologies (FM&NT), and to Riga.

In 2018, Latvia celebrates a hundred years since it became an independent state. Our neighbours - Estonia and Lithuania – are celebrating their centenaries of statehood as well. With festivities at home and all around the world, the Baltic countries will present the best they can offer in culture, lifestyle, and innovation. The arranged FM&NT-2018 conference on advanced materials and nanotechnologies falls under materials scientist's contribution in this year of the Baltic countries national anniversaries.

This conference is a continuation of annual meetings, first of which was organized in 2006 by the Institute of Solid State Physics, University of Latvia (ISSP UL) in Riga. Since 2013 FM&NT conferences turned over a new page – becoming a common conference of all three Baltic countries. Now it is being organized periodical by the ISSP of University of Latvia, University of Tartu, and Vilnius University. FM&NT is also a tribute to 40ty year jubilee of the ISSP UL and Centenary celebration of the University of Latvia in 2019.

The purpose of the conference is to bring together materials scientists, physicists, chemists, research staff, engineers, as well as experts in a wide range of the most demanding application areas, and students from universities, research institutes and related industrial companies. The conference topics include: Optical materials; Nanocomposites and ceramics; Thin films and coatings; Energy harvesting and storage; Electronic and photonic devices and yet more. 6 plenary talks, 19 invited talks, 37 oral presentations and over 130 posters of high scientific quality will be given at the conference. The joint event will also provide a platform for the future collaboration promoting interdisciplinary research.

The FM&NT-2018 conference will take place in Radisson Blu Latvia Conference & Spa Hotel in Riga. The Conference dinner and excursion will be held in Riga Motor Museum. The museum showcases more than a hundred unique antique vehicles and the collection is enriched with several significant acquisitions. Exploration the world of vehicles and their history of development could have some added scientific value for participants, e.g. to rouse new ideas on development of automotive batteries or other accessories, sensors and actuators for diagnostics and for realizing artificial intelligence prospects.

I wish to thank International Organizing and Program Committees, as well as Local Committees members for hard working preparing the Conference.

Thank you all for coming and I wish you most successful and pleasurable conference!

Andris Sternberg,
Chairman of FM&NT-2018
Institute of Solid State Physics, University of Latvia, Riga, Latvia

SCIENTIFIC TOPICS OF THE FM&NT-2018

THEORY:

Theory and computational material science by atomistic scale modelling of technologically important materials and devices

FUNCTIONAL MATERIALS:

Functional (inorganic, organic and hybrid) materials for electronics and photonics

NANO:

Progressive methods, technologies and design for production, investigation of nano - particles, tubes, composites, core-shell structures; 3-D printing, thin films and coatings

ENERGY:

Perspective materials and technologies for harvesting and storage of renewable energy: hydrogen, fuel cells, photovoltaics, piezoelectric, thermoelectric, LED and OLEDs, and developing of diverse energy systems.

LIST OF PREVIOUS FM&NT CONFERENCES

Riga (Latvia)	2006	
Riga (Latvia)	2007	
Riga (Latvia)	2008	
Riga (Latvia)	2009	
Riga (Latvia)	2010	
Riga (Latvia)	2011	
Riga (Latvia)	2012	
Tartu (Estonia)	2013	
Riga (Latvia)	2014	Joint RCBJSF and FM&NT Symposium
Vilnius (Lithuania)	2015	
Tartu (Estonia)	2017	

FM&NT-2018 COMMITTEES

Conference Chairman: Dr.habil. Andris Sternberg

FM&NT INTERNATIONAL ORGANIZING COMMITTEE

- Prof. Jūras Banys, Lithuania
- Prof. Antonio Bianconi, Italy
- Prof. emeritus Niels Egede Christensen, Denmark
- Prof. Robert Evarestov, Russia
- Prof. Claes-Göran Granqvist, Sweden
- Prof. Marco Kirm, Estonia
- Dr. Jiri Kulda, France
- Prof. Ergo Nõmmiste, Estonia
- Dr. Toomas Plank, Estonia
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- Dr. Linards Skuja
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- Dr. Andris Sternberg
- Dr. Qin Wang

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Committees sincerely hope that the FM&NT-2018 conference will give all the participants new insights into the wide spread development of functional materials and nanotechnologies, will enhance the circulation of information released at the meeting, and will bring new friends, contacts and common projects!

Thank you all for coming and we wish you successful and enjoyable conference.

USEFUL CONTACT PHONES

Conference chairman: Dr.habil.phys. Andris Sternberg (mobile)	+371 26183061
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Radisson Blu Latvia Conference & Spa Hotel	+371 67772222

ORGANIZERS:

INSTITUTE OF SOLID STATE PHYSICS
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IOP Publishing

Taylor & Francis
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FM&NT-2018 AGENDA AT A GLANCE

October 2	
16:00	**Registration**
17:00 18:30	**Welcome party**

Plenary - 50 min

Invited - 30 min

Oral - 20 min

- **Synchrotron and Neutron facilities**
- **Radiation effects & Scintillators**
- **Optical materials**
- **Thin films**
- **Ferroelectrics**
- **Nanocomposites and ceramics**
- **Electronic, photonic and magnetic materials and devices**
- **International cooperation projects**
- **Energy**
- **Nanomaterials**

October 3			
8:30	**Registration**		
	Beta Hall		
8:50	**Techincal information**		
9:00	**Opening - Conference chairman A.Sternberg, D. Stepanovs (Ministry of Education and Science), V. Seglins (University of Latvia), Marco Kirm (University of Tartu), Juras Banys (University of Vilnius)**		
9:20	**Andreas Schreyer**		
10:10	**Christina Trautmann**		
11:00	**Coffee 11:00 - 11:30**		
	Beta hall 1		**Beta hall 2**
11:30	K. Klementiev	11:30	R. Evarestov
12:00	M. Kirm	12:00	Y.Zhydachevskyy
12:30	A.Frenkel	12:30	V. Nagirnyi
13:00	A. Anspoks	13:00	A. Trukhanov
13:20	M. Klepka	13:20	V. Kuzovkov
13:40	**Lunch 13:40 - 14:40**		
	Beta hall 1		**Beta hall 2**
14:40	A. Bagaturyants	14:40	E. Zschech
15:10	M. Popova	15:10	L. Österlund
15:40	I. Norrbo	15:40	I. Oja Acik
16:00	L. Trinkler	16:00	H. Seemen
16:20	J. Spigulis	16:20	M. Zubkins
16:40	**Photo &Coffee & Snacks 16:40 - 17:20**		
17:20	**Poster session 17:20 - 19:00**		

Ocotber 4			
8:30	**Registration**		
	Beta Hall		
9:00	**Techincal information**		
9:10	**Andrei Kholkin**		
10:10	**Aharon Gedanken**		
10:50	**Coffee 10:50 - 11:20**		
	Beta hall 1		**Beta hall 2**
11:20	V. Shur	11:20	A. Kareiva
11:50	V. Shvartsman	11:50	S. Kulkova
12:20	E. Politova	12:10	A. Antuzevics
12:40	P. Czaja	12:30	E. Ryklina
13:00	P. Ščajev	12:50	I. Khmelevskaya
13:20	R. Eglitis	13:10	B. Kodatski
		13:30	C. Saikaew
13:50	**Lunch 13:50 - 14:50**		
	Beta hall 1		**Beta hall 2**
14:50	J. Banys	14:50	A. Sternberg
15:20	A. Salak	15:30	T. Plank
15:50	O. Malyshkina	15:50	V. Kisand
16:10	E. Makagon	16:10	A. Popov
16:40	**Excursion & Conference dinner at the Riga Motor Museum 16:40 - 21:30**		

October 5			
8:30	**Registration**		
9:00	**Coffee 9:00 - 9:30**		
	Beta hall 1		**Beta hall 2**
9:30	J. Pflaum	9:30	A. Lipovski
10:00	L. Vieira	10:00	M. Chou
10:30	G. Niklasson	10:30	L. Valkunas
10:50	E. Kotomin	10:50	A. Bandura
11:10	A. Yaremchenko	11:10	G. Kunakova
11:30	Y. Zhukovskii	11:30	E. Trukhanova
11:50	R. Bartali	11:50	G. Gorokhov
12:10	**Lunch 12:10 - 13:00**		
	Beta Hall		
13:00	**Maija Kuklja**		
13:50	**Peter Kazansky**		
14:40	**Closing - Rector of the University of Latvia I. Muiznieks, Conference chairman A.Sternberg**		
15:00	**Goodbye refreshments 15:00 - 16:00**		

			Tuesday, October 2
16:00 – 17:00	REGISTRATION		
17:00 – 18:30	WELCOME PARTY		
			Wednesday, October 3
08:00 – 08:50	REGISTRATION		
BETA HALL			
Beta hall	**OPENING**		
Chairperson: Andris Sternberg			
09:00 – 09:05	Andris Sternberg	Chairman of the Conference, Institute of Solid State Physics, University of Latvia	
09:05 – 09:10	Dmitrijs Stepanovs	Deputy State Secretary and Director of the Higher Education, Science and Innovation Department at Ministry of Education and Science, Latvia	
09:10 – 09:13	Valdis Segliņš	Vice Rector – University of Latvia, Latvia	
09:13 – 09:16	Marco Kirm	Professor – Institute of Physics, University of Tartu, Estonia	
09:16– 09:19	Jūras Banys	Professor – Faculty of Physics, Vilnius University, Lithuania	
Beta hall	**PLENARY SESSION**		
09:20 – 10:10	Andreas Schreyer	ESS and Its Contributions to Future Functional Materials and Nanotechnology	PL-1
10:10 – 11:00	Christina Trautmann	Material Science and Nanostructures Produced with GeV Heavy Ions	PL-2
11:00 – 11:30	**COFFEE**		
BETA HALL 1			
Beta hall 1	**SYNCHROTRON AND NEUTRON FACILITIES**		
Chairperson: Jiri Kulda			
11:30 – 12:00	Konstantin Klementiev	MAX IV Laboratory in Lund, Sweden: Research Portfolio, Present Status Expected Performance	INV-1
12:00 – 12:30	Marco Kirm	A Role of Large Scale Facilities in the Development of Novel Functional Materials	INV-2
12:30 – 13:00	Anatoly Frenkel	A Neural Network Approach for Structural Characterization of Metal Nanoparticles and Clusters	INV-3
13:00 – 13:20	Andris Anspoks	Temperature Dependent Local Atomic Structure Studies of Bulk and Nanocrystalline CuO Using X-ray Absorption Spectroscopy	OR-1
13:20 – 13:40	Marcin Klepka	Studies of Non-crystalline Metal-organic Ligand Complexes Using Methodology Based on XAFS	OR-2

BETA HALL 2			
Beta hall 2	**RADIATION EFFECTS & SCINTILLATORS**		
Chairperson: Eugene Kotomin			
11:30 – 12:00	Robert Evarestov	Theoretical Modeling of Point Defects in Crystals	INV-4
12:00 – 12:30	Yaroslav Zhdachevskyy	Photoluminescence Quantum Yield as a Test of Quantum Cutting Processes in Down-Converting Phosphors	INV-5
12:30 – 13:00	Vitali Nagirnyi	New Features of Hot Intraband Luminescence for Fast Timing	INV-6
13:00 – 13:20	Alex Trukhanov	New Functional Material for Semiconductor Devices Protection against Electron Radiation	OR-3
13:20 – 13:40	Vladimir Kuzovkov	Understanding of the Kinetics of Defect Annealing in Heavily Irradiated Binary and Complex Oxides – Disordering Effects	OR-4
13:40 – 14:40	**LUNCH**		
BETA HALL 1			
Beta hall 1	**OPTICAL MATERIALS**		
Chairperson: Vitali Nagirnyi			
14:40 – 15:10	Alexander Bagatyurants	Theoretical Modelling in Nanophotonics	INV-7
15:10 – 15:40	Marina Popova	Crystals for Optical Quantum Memory	INV-8
15:40 – 16:00	Isabella Norrbo	Luminescence in Synthetic Hackmanites	OR-5
16:00 – 16:20	Laima Trinkler	280 nm Emission Band in LiGaO$_2$	OR-6
16:20 – 16:40	Janis Spigulis	Human Skin as an Optical Material	OR-7
BETA HALL 2			
Beta hall 2	**THIN FILMS**		
Chairperson: Juris Purans			
14:40 – 15:10	Ehrenfried Zschech	Application of X-ray Microcopy in Materials Science and Nanotechnology	INV-9
15:10 – 15:40	Lars Österlund	Novel Self-Cleaning, Air Cleaning and Thermochromic Films for the Built Environment	INV-10
15:40 – 16:00	Ilona Oja Acik	Photocatalytic TiO$_2$ Thin Films for Air Cleaning Applications	OR-8
16:00 – 16:20	Helina Seemen	The Properties of Atomic Layer Deposited Zirconium and Cobalt Oxide Nanolaminates	OR-9
16:20 – 16:40	Martins Zubkins	Thin Film Deposition by Magnetron Sputtering at Cryogenic Substrate Temperatures	OR-10
16:50 – 17:20	**PHOTO & COFFEE & SNACKS**		
17:20 – 19:00	**POSTER SESSION**		

Thursday, October 4

08:30 – 09:00	REGISTRATION		
BETA HALL			
09:00 – 09:10	TECHNICAL INFORMATION		
Beta hall	**PLENARY SESSION**		
Chairperson: Andris Sternberg			
09:10 – 10:00	Andrei Kholkin	Nanoscale Piezoelectric Materials: Structure, Properties, Applications	PL-3
10:00 – 10:50	Aharon Gedanken	Making the Hospital a Safer Place by the Sonochemical coating of all its Textiles and Medical Devices with Antibacterial Nanoparticles	PL-4
10:50 – 11:20	**COFFEE**		
BETA HALL 1			
Beta hall 1	**FERROELECTRICS**		
Chairperson: Juras Banys			
11:20 – 11:50	Vladimir Shur	Shapes of Isolated Domains in Uniaxial Ferroelectrics	INV-11
11:50 – 12:20	Vladimir Shvartsman	Electrocaloric Effect in Barium Titanate Based Ceramics and Single Crystals	INV-12
12:20 – 12:40	Ekaterina Politova	Lead-free Ceramics on the Base of Sodium-Bismuth Titanate and Sodium-Potassium Niobate	OR-11
12:40 – 13:00	Piotr Czaja	Influence of Powder Grinding Time on the Microstructure of the Lead-free $K_{0.5}Bi_{0.5}TiO_3$ Ceramics	OR-12
13:00 – 13:20	Patrik Ščajev	Dispersion Carrier Recombination and Diffusion in $MAPbI_3$ and $MAPbBr_3$ Perovskite Crystals in Wide Excitation Range	OR-13
13:20 – 13:40	Roberts Eglitis	Ab initio Calculations of ABO_3 Perovskite (001), (011) and (111) Surfaces, Interfaces and Defects Therein	OR-14
BETA HALL 2			
Beta hall 2	**NANOCOMPOSITES AND CERAMICS**		
Chairperson: Anatoly Frenkel			
11:20 – 11:50	Aivaras Kareiva	Multicomponent Metal Oxide Systems for Optical and Magnetic Applications	INV-13
11:50 – 12:10	Svetlana Kulkova	Oxygen Diffusion in Ti-Al Alloys	OR-15
12:10 – 12:30	Andris Antuzevics	Electron Paramagnetic Resonance in Glass Ceramics	OR-16
12:30 – 12:50	Elena Ryklina	Effect of Grain Size on Microstructure, Transformation Behavior and Functional Properties of Ti-Ni Shape Memory Alloy	OR-17

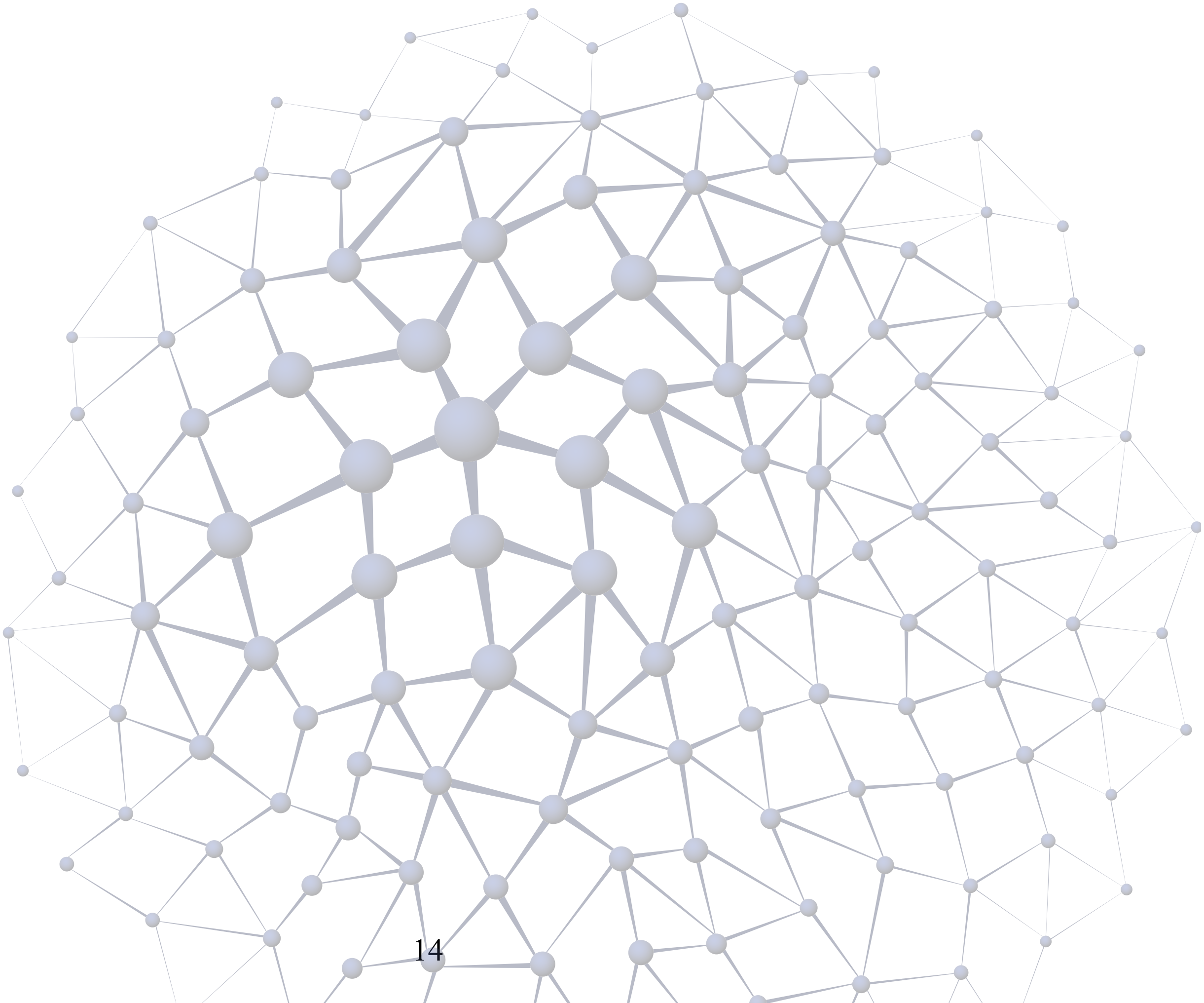
BETA HALL 2			
12:50 – 13:10	Irina Khmelevskaya	Features of Nanostructure and Functional Properties Formation in Ti-Ni SMA by ECAP Method Under Quasi-continuous Mode	OR-18
13:10 – 13:30	Bogdan Kodatski	Nematic Mesomorphous Systems Based on Dispersions of Carbon Nanotubes and Mineral Particles	OR-19
13:30 – 13:50	Charnnarong Saikaew	Influences of Sputtering Process Factors on Wear Resistance of TiN Coated on a Machine Component	OR-19
13:50 – 14:50	**LUNCH**		
BETA HALL 1			
Beta hall 1	**ELECTRONIC, PHOTONIC AND MAGNETIC MATERIALS AND DEVICES**		
Chairperson: Andrei Kholkin			
14:50 – 15:20	Jūras Banys	Dielectric Response of the Methylammonium Lead Halide Solar Cell Absorbers	INV-14
15:20 – 15:50	Andrei Salak	Tuneable Magnetic Co(II)-Containing Layered Double Hydroxides	INV-15
15:50 – 16:10	Olga Malyshkina	Determination of the Electron Effective Mass for n-type Germanium by the Low-frequency Impedance	OR-21
16:10 – 16:30	Evgeniy Makagon	Ceria-based electro-chemo-mechanical actuator with Ti/ $Ce_{1-x}Gd_xO_{2-x/2}$ composite contacts	OR-22
BETA HALL 2			
Beta hall 2	**INTERNATIONAL COOPERATION PROJECTS**		
Chairperson: Marco Kirm			
14:50 – 15:10	Andris Sternberg	CAMART^2 - Regional Development Opportunity	OR-23
15:10 – 15:30	Toomas Plank	Solar Energy with New Generation Power Electronics Solutions	OR-24
15:30 – 15:50	Kisand Vambola	Baltic TRAM – a Network of Industrial Research Centers Providing Analytical Services for Business Innovation in the Baltic Sea Region	OR-25
15:50 – 16:10	Anatoli Popov	Advanced Materials and Technologies in Fusion Research: An Overview and Some Recent Results from Latvian EUROfusion Laboratory	OR-26
16:40 – 21:30	**EXCURSION AND CONFERENCE BANQUET AT THE RIGA MOTOR MUSEUM**		

Friday, October 5

09:00 – 09:30	REGISTRATION & COFFEE		
BETA HALL 1			
Beta hall 1	**ENERGY**		
Chairperson: Martins Rutkis			
09:30 –10:00	Jens Pflaum	Low-Dimensional Organic Conductors for Thermoelectric Applications	INV-16
10:00 – 10:30	Luciana Vieira	Functional Materials for the CO$_2$-based Electrosynthesis of Ethylene Oxide	INV-17
10:30 – 10:50	Gunnar A. Niklasson	Impedance Spectroscopy of Water Splitting Reactions on Nanostructured Metal-based Catalysts	OR-27
10:50 – 11:10	Eugene Kotomin	First Principles Calculations of Perovskite Solid Solutions for Fuel Cells	OR-28
11:10 – 11:30	Aleksey Yaremchenko	LaNiO$_3$-based Oxygen Electrodes for Solid Oxide Electrolysis Cells	OR-29
11:30 – 11:50	Yuri Zhukovskii	First Principles Evaluation of Photocatalytic Suitability of 2H Structured and [0001] Oriented Graphene-like WS$_2$ Nanosheets and Nanotubes	OR-30
11:50 – 12:10	Ruben Bartali	Hydrogen Production by Water-Hydrolysis using Graphene Powder Coated with Magnesium	OR-31
12:10 – 13:00	**LUNCH**		
BETA HALL 2			
Beta hall 2	**NANOMATERIALS**		
Chairperson: Konstantin Klementiev			
09:30 –10:00	Andrey Lipovskii	Plasmonic Nanoislands on Glass: Formation and Properties	INV-18
10:00 – 10:30	Mitch Chou	Preparation and Characterization of Heteroepitaxial Cu$_2$O Thin Film and Devices on Metallic Substrates	INV-19
10:30 – 10:50	Leonas Valkunas	Relaxation Pathways in Semiconducting Carbon Nanotubes	OR-32
10:50 – 11:10	Andrei Bandura	New Three-body Force-field for Calculation of the Thermodynamic Properties of MoS$_2$ Nanolayers and Nanotubes	OR-33
11:10 – 11:30	Gunta Kunakova	Studies of Magnetotransport and Josephson Supercurrent in Topological Insulator Nanoribbons	OR-34
11:30 – 11:50	Ekaterina Trukhanova	Synthesis and Magnetotransport Properties of the Multilayered Quasi-one-dimensional Nanostructures	OR-35
11:50 – 12:10	Gleb Gorokhov	Carbon Nanotubes vs Graphene Nanoplatelets for 3D-printable Composites	OR-36
12:10 – 13:00	**LUNCH**		

BETA HALL

Beta hall	**PLENARY SESSION**		
Chairperson: Andris Sternberg			
13:00 – 13:50	Maija Kuklja	Understanding Chemical Reactions Triggered by Defects on Energetic Materials and Interfaces. Insight from Quantum Chemistry	PL-5
13:50 – 14:40	Peter Kazansky	Advancing the art of femtosecond laser writing	PL-6
Beta hall	**CLOSING OF THE CONFERENCE**		
14:40 – 14:50	Indrikis Muiznieks	Rector of the University of Latvia	
14:50 – 15:00	Andris Sternberg	Chairman of the Conference, Institute of Solid State Physics, University of Latvia	
15:00 – 17:00	**GOODBYE REFRESHMENTS**		



POSTER PRESENTATIONS

PO-1	Comparative First-Principles Calculations of ZrS_2 and HfS_2-based Nanotubes	Anton Domnin
PO-2	Comparative Study of Phonons and Thermodynamic Properties of MoS_2 and WS_2 Nanotubes	Robert Evarestov; Andrei Bandura
PO-3	Atomistic Scale Modelling of Modern Materials using ACELAN Package	Roman Gruzdev
PO-4	The Influence of Impurities on the Formation Energies of Point Defects in Ti-Al Alloys	Alexander Bakulin
PO-5	Influence of Fluorine and Oxygen Adsorption on Electronic Structure of InSb(111) Surface	Artem Fuks
PO-6	CO_2 Adsorption on Mixed Ionic-Electronic Conducting Membranes	Denis Gryaznov
PO-7	Negative Thermal Expansion of ScF_3: First Principles vs Empirical Molecular Dynamics	Dmitry Bocharov
PO-8	Simulation of the Band Structure and Density of States of the Nanocrystal NaCl	Lyudmila Myasnikova
PO-9	First Principles Calculations for Polar $YAlO_3$ (001) Surfaces	Roberts Eglitis
PO-10	Quantum Paraelectric State in $(Pb_ySn_{1-y})_2P_2S_6$ Crystals	Ilona Zamaraite
PO-11	Modeling of F-type Centers Thermal Annealing in Neutron Irradiated and Thermochemically Reduced BeO	Vladimir Kuzovkov
PO-12	Lattice Dynamics of White Phosphorus	Janis Brokans
PO-13	Structural and Electronic Properties of pure and Ce^{3+}doped β-$NaYF_4$	Aleksandrs Platonenko
PO-14	Stability and Mechanical Properties of Al_2O_3/Ti_3Al Interface	Sergey S. Kulkov
PO-15	Ab Initio Simulation of $(Ba,Sr/Ca)TiO_3$ Composite Perovskites	Guntars Zvejnieks
PO-16	Magnetic Properties of Solid Solutions $LaGa_{1-x}FexO_3$ and $LaAl_{1-x}Fe_xO_3$: First-Principles Study	Mariia Sapova
PO-17	Revealing Conduction Pathways in Solid Lithium Electrolytes by Total Scattering X-ray and Neutron Diffraction Measurements Using Molecular Dynamics Simulation and RMCPOW Methods	László Temleitner
PO-18	Dipole-induced Disorder in Quasi-Equilibrium Assemblies	Eugene Kotomin
PO-19	Computer Simulation of Cu_n@graphene (0001) Nanostructures for the Electrocatalytic Production of C_2H_4O	Sergei Piskunov
PO-20	Improved Electrochemical Performances Derived From Synergistic Effect of Reduced Graphene Oxide and TiO_2/Fe_2O_3 in Various Proportions Served as Lithium-Ion Battery Anode	Kaspars Kaprans
PO-21	Characteristics of Polymer Electrolyte Membrane Impedance Analysis	Deniss Fedorenko
PO-22	Photo-catalytic and Electro-catalytic CO_2 Reformation – Reactions and Efficiencies in Separate and Combined Processes (Review)	Ainars Knoks
PO-23	Ternary Nafion©-Graphene-Cu Composite for Electrochemical Reduction of CO_2 to Ethylene	Julija Hodakovska
PO-24	1,3-Dimethylimidazolium Dimethyl Phosphate and SPEEK based Composite Proton Conducting Membranes	Marta Kāne
PO-25	Nanostructured Nitrogenated Carbon Materials as Promoters in Hydrogen Energy Technologies	Janis Kleperis
PO-26	Gas Separation Using WO_3/NiOOH Red-Ox Mediator Pair in Four Electrode, Dual Chamber Electrolysis Cell	Martins Vanags

PO-27	Nanomaterials and Key Technologies for Bio-H_2 Separation	Ilze Dimanta
PO-28	The Impact of Zirconium Phosphate Content on Proton Conductivity of Composite Polymer Electrolyte	Einars Sprugis
PO-29	Preparation of ZnO Modified TiO_2 Nanoporous Coatings and Their Photocatalytic Properties	Reinis Drunka
PO-30	Photonic Sensor for Distinguishing Dead and Alive Bacteria Content for Monitoring of Decontamination Efficiency	Ott Rebane
PO-31	Defects Creation in Undoped and Ce-doped $Gd_3(Ga,Al)_5O_{12}$ Crystals under Irradiation in the Gd^{3+} related Absorption Bands	Svetlana Zazubovich
PO-32	EPR Spectroscopy of Mn^{4+}Doped Germanium Garnet	Marek Oja
PO-33	Pressure-Induced Structural Changes in Alpha-MoO_3 Probed by X-ray Absorption Spectroscopy	Inga Jonane
PO-34	Raman Spectroscopy Studies of Temperature Dependent Ferroelectric Instability in $SrTi^{18}O_3$	Nina Mironova-Ulmane
PO-35	Depth Profiles of Damage in MgO Single Crystals Irradiated with Swift Heavy Ions	Ilze Manika
PO-36	Effect of In on the ZnO Powders Morphology and Microstructure Evolution of ZnO:In Ceramics as a Material for Scintillators	Faina Muktepavela
PO-37	Vibrational Spectra and Lattice Dynamics in the β Form of White Phosphorus	George Chikvaidze
PO-38	Float Zone Single Crystals for Testing Rods, Pulled Under Electron Beam Heating	Anatoly Kravtsov
PO-39	Production of Phosphorescent Coatings Using Plasma Electrolytic Oxidation Method	Krišjānis Auziņš
PO-40	Permittivity Increase of Carbon Black/Silicone Oil Suspension Induced by Electric Field	Kaspars Ozols
PO-41	Determination of Molecular Structure of Schiff Base Complexes with Cu Ions	Diana Kalinowska
PO-42	Effect of Composition of Steel and Holding Time on the GB Wetting by Copper	Dheeraj Varanasi
PO-43	Deuterium Concentrations in Austenitic Stainless Steel by Deuterium Irradiation. Effects of Temperature Irradiation	Oleksandr Morozov
PO-44	Temperature Range of Helium Retention From Austenitic Stainless Steel Implanted Helium at 600 K	Viktoria Seliukova
PO-45	Yttrium Oxyhydrides as a New Family of Mixed-Anion Functional Materials	Evgenii Strugovshchikov
PO-46	Reorganization Energy Quality Tested by Statistics	Igors Mihailovs
PO-47	Anisotropy of Singlet Oxygen Luminescence in Silica	Linards Skuja
PO-48	Luminescent Characteristics of Magnesium Aluminate Spinel of Different sStoichiometry	Gatis Prieditis
PO-49	Single Step Preparation of Phosphorescent Coating on Aluminum	Aleksejs Zolotarjovs
PO-50	Optical Investigation of the OH- Groups in the Layers of $LiNbO_3$ Crystals Formed by Copper Ions Diffusion	Dmytro Sugak
PO-51	Luminescence Properties and Ddecay Kinetics of Mn^{2+} and Eu^{3+} Ions in $MgGa_2O_4$ and $ZnGa_2O_4$ Ceramics	Dmytro Sugak
PO-52	Time Resolved Pulsed OSL Readout of Ceramic YAP:Mn Detectors	Yaroslav Zhydachevskyy

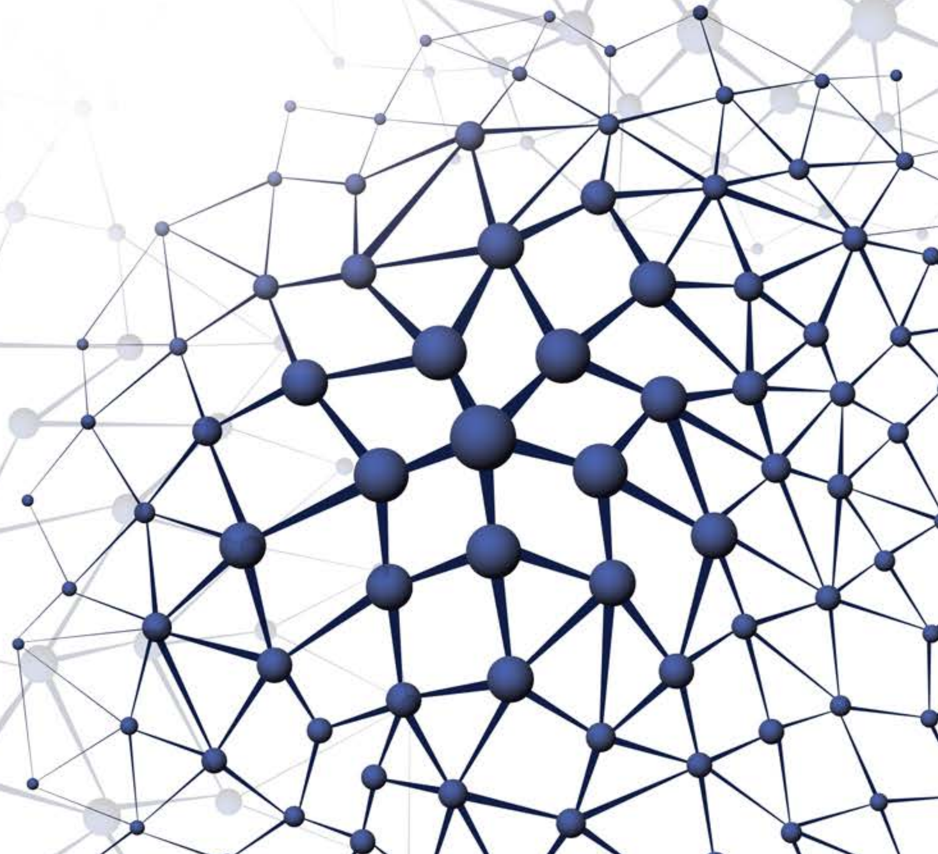
PO-53	Radiation Impurity Defects in the Activated Potassium Sulphate Crystals	Elmira Mussenova
PO-54	Luminescence of K_2SO_4 Crystals Doped by Ions of Divalent Rare-earth Elements	Ainura Tussupbekova
PO-55	Nanoporous Characterization of Modified Humidity-Sensitive MgO-Al_2O_3 Ceramics by Positron Annihilation Lifetime Spectroscopy Method	Anatoli Popov
PO-56	Structural Investigation of Crystallized Ge-Ga-Se Chalcogenide Glasses	Halyna Klym
PO-57	Wavefront Recovery From Intensity Measurements Using a Single Amplitude Modulating Mask	Varis Karitāns
PO-58	Enhancement of Photosensitivity in Azo-Epoxy Resists for Direct Holographic Recording	Jelena Mikelsone
PO-59	Photoinduced Mass Transport in Amorphous Chalcogenide and Azobenzene Organic Materials	Janis Teteris
PO-60	Improvement of Diffraction Parameters in Surface Relief Holograms	Mara Reinfelde
PO-61	Search for Defects in $SrAl_2O_4$:Eu,Dy Material	Virgīnija Vītola
PO-62	Tailoring of Thermoelectric Properties of Bi_2Se_3 Thin Films by Adjustment of Dopant Concentration	Jana Andzane
PO-63	Thermoelectrical Properties of NBT Ceramics	Kamila Kluczewska
PO-64	Effects of CuO Doping on Structure, Microstructure and Dielectric Properties of $BaTiO_3$-$PbTiO_3$ Solid Solution	Barbara Garbarz-Glos
PO-65	The Effect of Sr Modification on Mechanical Properties of $Na_{0.5}Bi_{0.5}TiO_3$ Ceramics	Jan Suchanicz
PO-66	Characterization of $SrTiO_3$ - $SrHfO_3$ Solid Solution by Dielectric Spectroscopy	Wojciech Bąk
PO-67	Preparation and Dielectric Properties of $(Na_{0.5}K_{0.5})NbO_3$ Ceramics with ZnO and CdO Addition	Grzegorz Klimkowski
PO-68	Effect of Cu Doping on the Electrical Properties of $Ba_{0.95}Pb_{0.05}TiO_3$ Ceramics by Means of Impedance Spectroscopy	Dorota Sitko
PO-69	Thermal Expansion and Polarization of $(1-x)PbNi_{1/3}Nb_{2/3}O_3-xPbTiO_3$ Solid Solutions	Anna Kalvane
PO-70	Dielectric Properties and AC Conductivities of $Bi_{1-x}Sm_xFeO_3$ Ceramics	Anna Kalvane
PO-71	Evolution of Domain Structure of $LiNbO_3$:ZnO Crystals During High Temperature Annealing	Maija Antonova
PO-72	Studies of Hydrogen Ion Bonds and Their Influence on Formation Structure of $LiNbO_3$:Mg and $LiNbO_3$:Zn Crystals	Maija Antonova
PO-73	Photoelectric Fields in Doped Lithium Niobate Crystals	Karlis Bormanis
PO-74	Optical Properties and Structure Particularities of $LiNbO_3$ Crystals Grown from Boron-Doped Melt	Karlis Bormanis
PO-75	Research of the Model of Lithium Niobate Cluster	Laura Eglite
PO-76	Grain Growth in $Na_{0.5}Bi_{0.5}TiO_3$-based Solid Solutions	Laura Eglite
PO-77	Effects of Strong Electric Fields on Polarization and Structural Properties Changes of 3d-ion Doped PLZT 8/65/35 Ceramic	Maris Kundzins
PO-78	Heat Capacity of Multiferroics $Bi_{1-x}Pr_xFeO_3$	Maris Kundzins
PO-79	Oxygen Isotope Exchange with oxides $La_{1-x}Sr_xCoO_{3-\delta}$	Natalia Porotnikova
PO-80	Electromechanical Properties of Some Relaxor-PT Solid Solutions	Sarunas Svirskas
PO-81	Dielectric Properties of $BaTiO_3$ Based Composites	Sergejus Balčiūnas

PO-82	Dielectric Response of ZIF-90 and UiO-66 Metal-Organic Frameworks under Different Gas Atmospheres	Robertas Grigalaitis
PO-83	Dielectric properties of PVDF-based barium titanate and nickel zinc ferrite flexible films	Robertas Grigalaitis
PO-84	Non-Linear Dielectric Spectroscopy of Mn-doped $PbMg_{1/3}Nb_{2/3}O_3$-0.1$PbTiO_3$	Dziugas Jablonskas
PO-85	Dielectric Investigations of Bismuth Niobate Manganate Ceramics	Juras Banys
PO-86	Ultra-low Percolation Threshold in Epoxy Resin – Onion-like Carbon Composites	Juras Banys
PO-87	Electrical Properties of Onion-like Carbon Composites	Ieva Kranauskaite
PO-88	Influence of Aluminosilicate Hollow Microspheres on the Electromagnetic Properties of MWCNT / PLA Composites	Darya Meisak
PO-89	Synthesis and Studying of Reduced Few-Layered Graphene Coatings in Gas Sensor Applications	Ingars Lukosevics
PO-90	Frequency Modulations in Electrochemical Exfoliation of FLG from Recycled Graphite	Peteris Lesnicenoks
PO-91	Mathematical Modeling and Parameter Optimization of the Enzyme Power Source for a Nano Drug Delivery System	Guntars Vaivars
PO-92	Nafion and polyaniline composite modification with Li and Mg ions	Stanislavs Lozkins
PO-93	AlN Nanopowders as Luminescent Markers for Biological Materials	Baiba Berzina
PO-94	Production of Variable Thickness Anodic Alumina Spacer for Metal-Insulator-Metal Optical Resonators	Daniels Jevdokimovs
PO-95	Up-Converting Nanoparticle Agglomeration Impact on Luminescence	Aleksejs Zolotarjovs
PO-96	Thermostimulated Luminescence Properties of Neutron, Electron and Thermochemically-reduced $Y_3Al_5O_{12}$	Edgars Elsts
PO-97	Cathodoluminescence Studies of Nanostructured AlN, AlN Nanotube/CsI Scintillator and AlN Nanotube/polymer Composites.	Alexandra Moskina
PO-98	Influence of Pressure and Temperature on X-ray Induced Photoreduction of Nanocrystalline CuO	Alexei Kuzmin
PO-99	Investigation of Plasmon Properties of Cu Nanoparticles in Various Solvents	Assylbek Zeinidenov
PO-100	Synthesis and Applications of Dense Plasmonic Nanoparticle Arrays on Porous Anodic Alumina Templates	Juris Prikulis
PO-101	Properties of CaF_2 and BaF_2 Nanofluorides Produced by Pulsed Electron Beam Evaporation	Vladislav Ilves
PO-102	Some Features of Surface-Ligand Interactions in Nanosized Fe_3O_4 Probed by Colloid Magnetometry	Mikhail Maiorov
PO-103	ZnO/WS_2 Nanowire Core/shell Heterostructures for Light Detection	Edgars Butanovs
PO-104	Influence of Inner Stresses on the Mechanical Properties of Fivefold Twinned Nanowires	Magnus Mets
PO-105	Electronic Processes in Doped ZnO Nanopowders	Larisa Grigorjeva
PO-106	Optical Properties of HfO_2 and HfO_2:Eu^{3+} Synthesized by Various Methods	Katrina Laganovska
PO-107	The Dependence of the Morphological Properties and Intrinsic Defects of HfO_2 Nanoparticles on the Selected Chemical Synthesis Method	Ivita Bite

PO-108	Magneto-Gravitational Separation of Nonmagnetic Materials in Electronic Waste	Viesturs Sints
PO-109	Carbon Aerogels as Nanomaterial for Supercapacitors	Alexander Ukshe
PO-110	Mass Recovery of Carbonated Fabrics of Glass Fibres after Isothermal Heating	Evalds Pentjuss
PO-111	Wood-based Nitrogen Doped Activated Carbons for Fuel Cells	Ance Plavniece
PO-112	Characterization of Conductive PEDOT:PSS Films Blended with SWCNTs and PVA	Guna Vugule
PO-113	Characterization of Bi_2O_3 Film in Compound with $MnFe_2O_3$ Nanoparticles	Mats Mikkor
PO-114	Structural Studies of Y-doped Iron Thin Films	Arturs Cintins
PO-115	TiO_2 Thin Films as Efficient Photocatalytic Material for Air Purification	Ibrahim Dündar
PO-116	Hardness and Modulus of Elasticity of Atomic Layer Deposited Al_2O_3-ZrO_2 Mixtures, Nanolaminates and Al-doped ZrO_2	Taivo Jõgiaas
PO-117	Determining the Hardness of Thin Oxide Coatings	Helle-Mai Piirsoo
PO-118	Mechanical and Optical Properties of HfO_2/ZrO_2 Nanolaminates Grown Using Atomic Layer Deposition	Mikk Kull
PO-119	Correlation Between Technological Regimes and Microstructure for Nanogranular Ni-Fe Films	Tatyana Zubar
PO-120	Specific Features of Magnetic Domain Structure in Epitaxial Ferrite-garnet Films with Planar Anisotropy	Alexandra Ivanova
PO-121	Ferroelectric Properties of Composite Films Based on Polystyrene	Ekaterina Barabanova
PO-122	Local Structure and Valence State of IrO Nanocrystalline and Amorphous Thin Film	Halil Arslan
PO-123	Optical Properties of Zinc-Iridium Oxide Thin Films	Vera Skvortsova
PO-124	GeSn Optoelectronic Properties by Nondestructive Characterization	Patrik Ščajev
PO-125	Magnetron Sputtering of Zn/Al Target by High Power Pulses in an Ar/O_2 Atmosphere and ZnO:Al Thin Films Deposition	Martins Zubkins
PO-126	Comprehensive Characterization of the Amorphous TaxOy Thin Films Deposited on Si and Glass	Krystyna Lawniczak-Jablonska
PO-127	Studies of Thermoelectric Properties of P3HT for 3D Printing Applications	Normunds Ralfs Strautnieks
PO-128	XPS Studies of [EMIM][BF4] Ionic Liquid Films	Mati Kook
PO-129	Photoluminescence and Electrical Properties of GaAs (111)A Epitaxial Layers Prepared by MOCVD	Krisjanis Smits
PO-130	Innovative Nanomaterials – Peculiarities of Formation of Strained Lead Selenide Nanolayers	Omar I. Davarashvili

PLENARY
AND INVITED SPEAKERS

International Conference Functional Materials and Nanotechnologies
'FMNT – 2018'



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Prof. Dr. Andreas Schreyer
European Spallation Source
Sweden

Prof. Dr. Andreas Schreyer is the Director for Science of the European Spallation Source (ESS) in Lund, Sweden since 2016. Before he joined ESS, he was head of the Institute of Materials Research at the Helmholtz-Zentrum Geesthacht, Germany and director of the German Engineering Materials Science Center (GEMS).
He also was the speaker of the Helmholtz research program "Research with Photons, Neutrons, and Ions" (PNI) coordinating the research with these three probes at all major large scale facilities in Germany. Prof. Schreyer teaches at Hamburg University since 2001. He received his venia legendi (professoral degree) in 2000 and his Ph.D in 1994 from the Ruhr-University Bochum. He was awarded a Heisenberg stipend of the Deutsche Forschungsgemeinschaft in 2000, a Feodor Lynen stipend of the Alexander von Humboldt foundation in 1998 and the prize for the best Ph.D. thesis of the Ruhr-University Bochum in physics in 1994.

Prof. Schreyer's research focuses on the analysis of lightweight materials, biomaterials, and magnetic nanostructures with X-rays and neutrons at large scale facilities. During his career he has been heavily involved with the design, construction and scientific use of scattering and imaging experiments at neutron and synchrotron sources. He has lead the construction of experiments at the Institute Laue Langevin in Grenoble, France, the PETRA III synchrotron storage ring at DESY, Hamburg and the Heinz-Maier-Leibnitz Zentrum in Garching, Germany. He now is responsible for the scientific experiments and infrastructure at the European Spallation Source in Lund, Sweden.

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Prof. Dr. Christina Trautmann

GSI Helmholtzzentrum and Technische Universität Darmstadt
Germany

Christina Trautmann is the head of the Materials Research Department of the GSI Helmholtz Center in Darmstadt (Germany) who operates a large scale accelerator facility for swift heavy ions.

Christina graduated in physics at the Technische Universität in Munich and received her PhD from the University of Frankfurt. Her research activities cover interaction processes of energetic, MeV to GeV, heavy ions with matter with focus on ion-beam induced modifications including defect and track formation in different material classes, performance limits of materials applied in high-dose environment and exposed to prolonged radiation (e.g., outer space, nuclear waste storage, reactor or accelerator environment, etc.) and the question how solids respond to the simultaneous exposure to pressure and ion beams. Together with her group and students from the TU Darmstadt, Christina operates several beamlines at the GSI accelerator facility and provides support to internal and external users for irradiation experiments that are dedicated to materials science including in-situ sample analysis by microscopic and spectroscopic techniques. She also promotes heavy ion beams for ion-track nanotechnology where the ion beam is used as tool for producing high-aspect-ratio micro- and nanostructures such as nanochannels and nanowires with tailored properties.

Christina teaches at the Technische Universität Darmstadt and is Editor of the Journal Nuclear Instruments and Methods in Physics Research, Section B, Beam Interactions with Materials and Atoms.

More information under: www.gsi.de/en/work/research/appamml/materials_research.htm

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Dr. Andrei Kholkin
Physics Department & CICECO, University of Aveiro
Portugal
School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg
Russia

Dr. Andrei Kholkin is one of the world leaders in the characterization and imaging of functional materials with the emphasis on ferroelectrics and multiferroics. He received his PhD degree in Solid State Physics from the A. F. Ioffe Physical-Technical Institute (St. Petersburg, Russia). Afterwards he held research positions in Leibniz Institute for Solid State and Materials Research (Germany), Swiss Federal Institute of Technology (Switzerland) and Rutgers University (USA). He is currently research coordinator and head of the advanced microscopy of functional materials laboratory of the CICECO-Aveiro Institute of Materials of the University of Aveiro (Portugal). His group develops multifunctional materials (including ferroelectrics, multiferroics and polar biomaterials) and scanning probe microscopy techniques for their study. He is a co-author of about 500 technical papers in this area including multiple reviews and book chapters. He was a coordinator of three European projects on functional materials and currently serves as an Associate Editor-in-Chief for the IEEE Transactions on Ultrasonics, Ferroelectrics and Frequency Control (TUFFC). He is a member of editorial boards of several scientific journals and serves in advisory boards of international conferences on ferroelectrics. He is a member of the Ferroelectric Committee of IEEE and was a recipient of the "Excellency" award from the Portuguese Foundation for Science and Technology. Dr. Kholkin is IEEE Fellow for his achievements in the development of electromechanical characterization tools and got a Ferroelectrics Recognition award from IEEE.

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Prof. Em. Aharon Gedanken
Department of Chemistry, Bar-Ilan University
Isarel

Prof. Em. Aharon Gedanken obtained his M. Sc. from Bar-Ilan University, and his Ph. D. degree from Tel Aviv University, Israel. After his postdoctoral research at USC in Los Angeles. He got a lecturer position at BIU on Oct. 1975. He spent two sabbatical years at AT&T Bell Laboratories in 1980-8l, and 1987-88 as well as a summer in 1984. He also has done research at NIDDK, NIH in the summers of 1989, 1990 and 1991. In 1994 he switched his research interest from Spectroscopy to Nanotechnology. His special synthetic methods of nanomaterials include: Sonochemistry, Microwave Superheating, Sonoelectrochemistry, and Reactions under Autogenic Pressure at Elevated Temperatures (RAPET). Since 2004 he is mostly focused on the applications of nanomaterials. **Gedanken has published 790 per-reviewed manuscripts in international journals, and has applied for 42 Patents. His H-Index is 86** according to the WEB of SCIENCE. Gedanken has served as the Department Chairman as well as the Dean of the Faculty of Exact Sciences at Bar-Ilan University. He is on the editorial boards of 5 international journals. He still leads a group of 13 research people. He was a partner in five EC (European Community) FP7 projects one of them, SONO, was coordinated by him. This project was announced by the EC as a "Success Story". He is a partner in PROTECT a textile project in Horizon 2020. He was the Israeli representative to the NMP (Nano, Materials, and Processes) committee of EC in FP7. He was awarded the prize of the Israel Vacuum Society in 2009 and the Israel Chemical Society for excellence in Research in Feb. 2013.

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Dr. Maija M. Kukla
Univrsity of Maryland
USA

PROFESSIONAL EXPERIENCE

Program Director (2002 – present), National Science Foundation, Arlington, VA

Office of the Director, Office of International Science and Engineering (02/2011 - present)
Develop national strategy, policy, and implementation of NSF programs and activities for enhancing international collaborative opportunities for US institutions, researchers, faculty, and students

Office of the Director, Office of Integrative Activities: (03/2008 – 02/2011)
Managed Experimental Program to Stimulate Competitive Research

Directorate for Mathematical and Physical Sciences, Division of Materials Research (12/02- 04/2008)
Designed and implemented national strategy and oversaw investments for materials research; managed multidisciplinary external research programs

EMBASSY SCIENCE FELLOW

US Embassy in Tbilisi, Georgia (10-11/2016)
Science Consultant to the US Government upon request of the State Department

- Evaluated work and portfolio of Shota Rustavely National Science Foundation of Georgia

US Embassy in Moscow, Russian Federation (05-07/2010)
Science Consultant to the US Government upon request of the State Department, http://moscow.usembassy.gov

- Prepared a holistic analysis of the status of nanotechnology in Russia to promote US-RF collaboration

RESEARCH INTERESTS

Condensed Matter Physics, Solid State Chemistry, and Materials Science, including but not limited to:

◊ Design of novel targeted materials; Energy storage and Conversion; Catalysis;
◊ Analytical theory and computer simulations; Development of multi-scale computational techniques;
◊ Ultra-fast processes in materials; Behavior of condensed matter in extreme conditions; Explosions;
◊ Molecular, Energetic, and Multifunctional materials; Defects, Deformations, Surfaces, and Interfaces;
◊ Modeling of the electronic structure, resonance phenomena, optics, and spectroscopy of solids;

PUBLICATIONS

- More than 140 peer-reviewed publications; 138 other technical reports
- 18 monographs, book chapters, invited and review articles
- 345 presentations at international conferences and professional meetings, including 167 invited lectures
- On October of 2017, based on web of science data, total citations – 2900, h-index – 34, i10-index – 65.

More information under: www.kuklagroup.umd.edu/about/index.html

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Prof. Peter G. Kazansky

Optoelectronics Research Centre, University of Southampton
United Kingdom

Peter G. Kazansky studied physics in Moscow State University and received Ph.D. under supervision of Nobel Laureate for the invention of laser A.M. Prokhorov from the General Physics Institute in 1985. He was awarded the Leninskii Komsomol Prize in 1989 for the pioneering work on "Circular photogalvanic effect in crystals". From 1989 to 1993 he led a group in the GPI, which unraveled the mystery of light-induced frequency doubling in glass. In 1992 he joined the ORC at the University of Southampton where since 2001 he is a professor pursuing his interests in new optical materials and phenomena. More recently he pioneered the field of ultrafast laser nanostructuring in glass leading to invention of "5D memory crystal," which holds a Guinness world record for the most durable data storage medium. From 2014 he is also a director of the International Centre of Laser Technologies in Mendeleev University of Technical Technologies. He served as Vice-Chair of the Committee on Glasses for Optoelectronics of International Commission on Glass and is a Fellow of Optical Society of America.

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Dr. Konstantin Klementiev
MAX IV Laboratory
Sweden

Konstantin Klementiev studied solid state physics in Moscow Engineering-Physics Institute and received his doctor's degree in 1998 with work in high temperature superconductivity and XAFS as the main experimental technique. While working as a postdoc and beamline scientist at DESY/Hamburg, he became more and more interested in methods and instrumentation in synchrotron radiation applications. Consequently, this interest resulted in the development of a ray-tracing and wave propagation toolkit xrt comprising physical models of synchrotron radiation sources and x-ray optics along with associated analysis tools (xrt.readthedocs.io). This development influenced and also gained from the design, assembly and commissioning of two XAFS/XES beamlines, first at Alba synchrotron and then at MAX IV, while he was working as beamline principal in Barcelona (2006-2013) and Lund (from 2013). His present focus is in bringing *Balder* – the XAFS/XES beamline of MAX IV – into full user operation.

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Prof. Marco Kirm

Institute of Physics, University of Tartu
Estonia

Marco Kirm, born 1965, is a professor of experimental physics at Institute of Physics, University of Tartu. He graduated University of Tartu cum laude as a physicist in 1991 and obtained his PhD„ Spectroscopy of highly charged ions, small molecules and solids under VUV excitation", supervised by Prof. Indrek Martinson, at Lund University in 1995. During 1997-2004 he worked at Hamburg University in the group of Prof. Georg Zimmerer as a post-doctoral researcher. As a beam-line scientist he was responsible for operation of the famous SUPERLUMI station (HASYLAB, DESY), designed for luminescence spectroscopy in VUV. Since 2004 after returning to Estonia, Marco Kirm has been in duties of a research director and director of Institute of Physics at University of Tartu. He was a Vice Rector for Research of University of Tartu during 2012-2017. In 2012 Marco Kirm was elected to the Latvian Academy of Sciences as a foreign member. In 2013 he received Baltic Assembly medal for the development of cooperation between Baltic States.

His research interests cover wide range of novel functional wide gap materials (incl. nanomaterials) applicable as LED phosphors, scintillators. He is also carrying out research on basic phenomena such as relaxation processes of electronic excitations and their dynamics by luminescence spectroscopy in wide time, temperature and energy range; ultrafast radiative processes (applications in PET tomography); creation of radiation defects in wide gap solids. He also focuses on novel optical diagnostics methods for thin dielectric films, optical materials and actively contributes to development luminescence spectroscopy setups under synchrotron radiation in Lund and Hamburg. His publication list includes 244 papers cited more than 3000 times (h-index 30) in the Web of Science.

In European Research Area he has been acting as an Estonian representative at the COST (Cooperation in Science and Technology, EU) in "Materials science, physics and nanosciences" domain committee. The INTERREG Baltic Sea Region innovation projects "Science Link" (2011-2014) and "Baltic Tram" (2016-2019) with a focus on access of large scale facilities and university labs by enterprises for their R&D are under the leadership of Marco Kirm in Estonia.

He has been organising various international scientific and educational events as chairperson: European Science Olympiade EUSO2016 (Tartu, May 7-14, 2016); 9th International Conference on Luminescent Detectors and Transformers of Ionizing Radiation – LUMDETR 2015 (20-25.09.2015, Tartu); Conference on functional materials and nanotechnologies FM&NT-2013 (in Tartu, April 21-24, 2013) and the most recent FM&NT-2017 held in Tartu April, 24 – 27, 2017.

Marco Kirm's continuously updated complete CV can be found at the Estonian Research Portal.

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Prof. Anatoly Frenkel
Department of Materials Science and Chemical Engineering,
Stony Brook University
Division of Chemistry, Brookhaven National Laboratory
USA

Anatoly Frenkel is a Professor in the Department of Materials Science and Chemical Engineering at the Stony Brook University and a Senior Chemist (Joint Appointment) at the Division of Chemistry, Brookhaven National Laboratory, having joined in the Fall of 2016. Prior to his appointment at SBU, he has held a number of different positions, including Associate and then appointed Full Professor and Chair, Physics Department at Yeshiva University, a Research Scientist and Principal Investigator in Materials Research Laboratory of the University of Illinois at Urbana-Champaign. He received M.Sc. degree from St. Petersburg University and Ph. D. degree from Tel Aviv University (with Prof. A. V. Voronel), all in Physics, followed by a postdoctoral appointment at the University of Washington (with Prof. E. A. Stern). His research interests focus on development and applications of in situ and operando synchrotron methods to solve a wide range of materials problems, with most recent emphasis on catalysis, electromechanical materials, filtration materials, quantum dots, physico-chemical properties of nanoparticles, as well as machine learning methods for structural analysis and design of nanomaterials. He is a founding Principal Investigator and the Spokesperson for the Synchrotron Catalysis Consortium at Brookhaven National Laboratory. He is a Fellow of the American Physical Society and a Fellow of the Empire Innovation Program at the New York State. He is the author of over 300 peer-reviewed publications, which have been cited > 14,000 times, and has given over 250 invited lectures at conferences and university, government and corporate laboratories.

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Prof. Robert A. Evarestov
Chemistry Department, Saint -Petersburg State University
Russia

Robert A. Evarestov graduated St. Petersburg State University as theoretical physicsist in 1960. He obtained his PhD in the Department of Theoretical Physics at St. Petersburg State University in 1964 (supervisor Prof. Marija Petrashen, coworker of Academician V.A.Fock), Habilitation degree -in the same Department in 1977 „ Molecular models in the electronic structure theory of crystals“. From 1968 he woks at the Department of Quantum Chemistry of St. Petersburg State University (Professor – from 1979). In 1990-1994 he was Director of the Chemistry Institute of St. Petersburg State University, in 1994-1998 he was First Vice Rector of St. Petersburg State University. Since 1999 till present time he is Head of Department of Quantum Chemistry of St. Petersburg State University.

His research interest cover symmetry of crystalline solids (the monograph „Site Symmetry in crystals„ has been published by Springer in 1993 , second edition in 1997). He is interested also by the application of quantum chemistry methods to perfect and defective crystals (the monograph „ Quantum Chemistry of Solids„ has been published by Springer in 2007 , second edition in 2012). Now his interests cover symmetry and quantum chemical study of monoperiodic nanostructures (nanotubes, nanowires). His monograph „ Theoretical Modeling of Inorganic Nanostructures. Symmetry and ab-initio calculations of nanolayers, nanotubes and nanowires“ has been published by Springer in 2015.

He is Foreign Member of Latvian Academy of Science (from 2005), Humboldt Foundation Awardee (1998). His publication list includes over 280 papers indexed in WOS and cited more than 2600 times , his Hirsh index is 28(Web of Science data, December 2016).

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Prof. Yaroslav Zhydachevskyy
Institute of Physics, Polish Academy of Sciences
Warsaw, Poland
Lviv Polytechnic National University
Lviv, Ukraine

RESEARCH INTERESTS

Optical and thermally activated spectroscopy of point defects, transition metal and rare earth ions in complex oxide crystals with garnet, perovskite and other types of structure. Energy and charge transfer processes between point defects and activator ions in the crystals. Photochromic properties of the crystals. Optical and luminescent properties of new solid-state laser, scintillator and phosphor materials. Thermally and optically stimulated luminescence for radiation dosimetry.

CURRENT RESEARCH ACTIVITIES

Research project of the European Regional Development Fund *(POIG 01.01.02-00-108/09), 2009-2014,* Topic: Novel Materials and Innovative Methods for Transformation and Monitoring of Energy (MIME), *Principal Investigator.*
NATO multi-year Science for Peace Project NUKR.SFPP 984649, 2015-2017, Topic: New Dosimetry for the Triage of People Exposed to Ionizing Radiation.
Project of the Ukrainian Ministry of Education and Science (No. 0117U004443, Acronym: Reader), 2017-2018, Topic: Development of a reader for individual passive OSL dosimetry of ionizing radiation based on YAP:Mn2+ crystals, *Project Leader.*
Project of the Polish National Science Centre 2015/17/B/ST5/01658, 2016-2019, Topic: Solar spectrum modification via down-conversion based on the ytterbium-doped oxides for photovoltaic applications, *Principal Investigator.*
Project of the Polish National Science Centre 2016/21/B/ST8/03200, 2017-2019, Topic: New scintillating screens based on single crystalline films of mixed oxides.
Project of the Polish National Science Centre 2017/25/B/ST8/02932, 2018-2020, Topic: Novel converting phosphors based on ceramics, films and epitaxial structures of mixed garnets for high-power white LEDs.

HONORS

Personal 6-month scholarship of the Polish Ministry of Education (2001 2002).
9-month scholarship (Leonhard – Euler program) funded by German Academic Exchange Service (DAAD) (2002).
NATO Advanced Fellowship for 8-month research stay in the Institute of Physics of the Polish Academy of Sciences, Warsaw, Poland (2003–2004).
Personal 2-year scholarship for young scientists from the Government of Ukraine (2007-2009).
Winner of the annual competition "Best young scientist of Lviv Polytechnic National University" in 2009.
Scientific Secretary of the International Conference on Oxide Materials for Electronic Engineering (OMEE-2009, OMEE-2012, OMEE-2014).
Guest Editor of selected volumes of *Acta Physica Polonica A and Solid State Phenomena* (2010-2018).
Invited lectures at conferences: *IWASOM-2006* (11-14 June, 2006, Gdańsk, Poland); E-MRS 2011 *Fall Meeting – Symposium H* (Sept. 19-23, 2011, Warsaw, Poland); *ICFM-2013* (Sept. 29 - Oct. 5, 2013 Haspra, Crimea, Ukraine); *IWASOM-2013* (Gdansk, Poland, 14-19 July, 2013), *ICSTAR-2018* (Sept. 23-25, 2018, Tirupati, India).

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Dr. Vitali Nagirnyi

Institute of Physics, University of Tartu

Estonia

Vitali Nagirnyi is a recognized expert in the field of time-resolved spectroscopy of wide gap solids under UV, VUV, XUV and X-irradiation. The main directions of his research are related to the investigation of the band structure of wide-gap crystals, relaxation processes and mutual interaction of electronic excitations (incl. the studies under extreme excitation conditions provided by modern free electron lasers and powerful short-wavelength fs-lasers), energy transfer from host matrices to intrinsic and extrinsic (e.g., impurity ions) luminescence centres. He has an extended research experience in working with various pulsed excitation sources such as synchrotron radiation (MAX-Lab, HASYLAB), free-electron laser FLASH (DESY), tunable OPO fs-laser systems (Laser Research Centre, University of Vilnius), electron guns (Tartu), and HHG devises (Saclay). V. Nagirnyi has been one of the leading researchers in a number of national grants awarded by Estonian Research Council and a Centre of Excellence project funded by European Commission and structural funding in Estonia. He has taken an active position in several international collaborations of INCO-COPERNICUS program, Crystal Clear Collaboration at CERN and in several COST actions (“Fast advanced Scintillator Timing” and “Advanced X-ray spatial and temporal metrology”). He is a recognized reviewer of journals Radiation Measurements, Journal of Luminescence, Vacuum, an Editorial Board member of Vacuum and has been a guest Editor of several IEEE TNS special issues. In his publication list, there are 133 papers according to Web of Science database. A complete CV of Vitali Nagirnyi can be found at the Estonian Research Portal.

e-mail: bagaturyants@gmail.com

Prof. Alexander Bagaturyants

Photochemistry Center RAS, Federal research center Crystallography and Photonics RAS
National Research Nuclear University MEPhI
Russia

EDUCATION:

1956 - 1962 D.I. Mendeleev Institute of Chemical Technology, Moscow, Department of Physical and Chemical Engineering, specialty: isotope separation and application technology.

SCIENTIFIC DEGREES

1968 PhD (Physical Chemistry), Institute of Organoelement Compounds, USSR Academy of Sciences, Moscow. PhD Thesis Title: "π-Electronic Structure of some Conjugated Systems with High Effective Charges on Atoms"

1987 Dr. Sci. (Physical Chemistry), N.N. Semenov Institute of Chemical Physics, USSR Academy of Sciences, Moscow. Doctoral Thesis Title: "Quantum Chemistry of Catalysis by Metal Complexes"

SCIENTIFIC TITLE

1992 Professor (Physical Chemistry), N.N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, Moscow.

CURRENT POSITION

Chief researcher, laboratory of Quantum Chemistry and Molecular Simulations, Photochemistry Center RAS, Federal State Institution "Federal research center Crystallography and Photonics Russian Academy of Science" (FRC Crystallography and photonics RAS) FRC C&P RAS Russian Academy of Sciences, ul. Novatorov 7a, Moscow, 119421 Russia, Moscow, full-time (main) job
Professor, Department of Condensed Matter Physics, National Research Nuclear University "MEPhI", Moscow, part-time (second) job.

RESEARCH INTERESTS

Quantum chemistry methods and applications. Ab initio quantum chemical calculations of molecules, clusters, and reaction paths.
First-principles DFT calculations of clusters, thin films, semiconductor surfaces, defects, and impurities;
Molecular simulations of molecular assemblies, supramolecular systems; and molecular aggregates.
Ab initio calculations of electronic spectra of organic molecules and metal organic complexes, molecular aggregates, and supramolecular systems using wave function and DFT methods.
Multiscale atomistic (molecular dynamics and quantum chemistry) simulations of organic and inorganic nanostructured materials for applications in sensing and photonics.

KEY WORDS

Quantum chemistry, molecular dynamics; ab initio, DFT, TDDFT, CASSCF, MCQDPT; electronic spectra, band shapes, line shapes; multiscale atomistic simulation; nano materials; chemical optical sensing, organic electronics and photonics

WEB SITES: www.photonics.ru; www.mephi.ru

LATEST BOOK:

Alexander Bagaturyants, Mikhail Vener, Multiscale Modeling in Nanophotonics. Materials and Simulation, Singapore, Pan Stanford Publishing, 2018, 274 pp.

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Prof. Marina Popova

Institute of Spectroscopy, Russian Academy of Sciences, Moscow, Troitsk
Russia

Marina Popova is Chief researcher and Head of the Fourier-Spectroscopy Laboratory in the Institute of Spectroscopy, Moscow. Her research interests include high-resolution spectroscopy, spectra of rare earths in crystals, spectroscopy of magnetic insulators, spectroscopy of multiferroics, phase transitions, hyperfine, interionic, electron-phonon interactions in crystals. At present, she is Leader of the joint Russian-Taiwanese project "Crystals for Quantum Memory", of several projects supported by Russian science foundations.

EDUCATION

Moscow Institute of Physics and Technology (Diploma with honors). The diploma work "Kinetics of the generation of a ruby laser with a concentric resonator" (1964) was performed at the Luminescence Laboratory of the Lebedev Physical Institute, RAS, under the supervision of A.M. Leontovich. Postgraduate study at MIPT and Lebedev Institute.

PHD DEGREE

The thesis "Dynamics of ruby laser" (supervisors M.D. Galanin and A.M. Leontovich) defended at the Lebedev Physical Institute (1968).
Dr. Sci. degree: The thesis "High-resoluion Fourier spectroscopy in studying crystals with rare-earth ions" defended in the Institute of Spectroscopy, RAS (1992).
Professor in optics: 2001.

EMPLOYMENT

The Institute of Spectroscopy, RAS

1975 – present The Latvian State University, the Problem Laboratory of Semiconductors. In 1969, she has assembled and

1968 – 1975 launched the first laser in the Baltic States. The study of multiphoton absorption in alkali-halide crystals, the lecture course "Lasers".

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Prof. Dr. Ehrenfried Zschech

Fraunhofer Institute for Ceramic Technologies and Systems, Dresden

Germany

Ehrenfried Zschech is Department Head for Microelectronic Materials and Nanoanalysis at the Fraunhofer Institute for Ceramic Technologies and Systems in Dresden, Germany, which he joined in 2009. His responsibilities include multi-scale materials characterization and reliability engineering. Ehrenfried Zschech received his Dr. rer. nat. degree from Technische Universität Dresden. After having spent four years as a project leader in the field of metal physics and reliability of microelectronic interconnects at Research Institute for Nonferrous Metals in Freiberg, he was appointed as a university teacher for ceramic materials at Freiberg University of Technology. In 1992, he joined the development department at Airbus in Bremen, where he managed the metal physics group and studied the laser-welding metallurgy of aluminum alloys. From 1997 to 2009, Ehrenfried Zschech managed the Materials Analysis Department and the Center for Complex Analysis at Advanced Micro Devices in Dresden. In this position, he was responsible for the analytical support for process control and technology development in leading-edge semiconductor manufacturing, as well as for physical failure analysis. He holds an adjunct professorship at Faculty of Chemistry of Warsaw University, Poland, as well as honorary professorships for Nanomaterials at Brandenburg University of Technology Cottbus and for Nanoanalysis at Technische Universität Dresden. Ehrenfried Zschech is member of the Board of Directors of the Materials Research Society (MRS) and Honorary Member of the Federation of the European Materials Societies (FEMS).

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Prof. Lars Österlund
Department of Engineering Sciences, The Ångström Laboratory,
Uppsala University
Sweden

Lars Österlund is Professor in solid state physics with specialization in environmental science and technology at Uppsala University. He is board member of the Uppsala Center for Photon Sciences, and is vice-chairman of the International Science Program. He is the co-founder of the Swedish Society of Vibrational Spectroscopy and was its president from 2010-2017. He is currently also CEO of a spin-off company developing micro-structured diamond waveguides.

Prof. Österlund has a PhD from 1997 from Chalmers, were his thesis work involved fundamental surface science studies of photo-induced surface reactions on single crystal surfaces employing a broad range of surface spectroscopic methods and reaction kinetic modelling. His postdoc research involved fundamental studies of surface reactions on single crystal surfaces employing scanning tunneling microscopy (STM), Monte-Carlo simulations of surface kinetics, and development of a high-pressure STM with atom-resolved imaging capabilities up to 1 bar and atomistic proof that was used to bridge the so called pressure gap in catalysis. A general theme of his current research is development of catalytic materials, including solar light responsive materials, such as photocatalytic materials, self-cleaning surface coatings, solid state gas-sensors and smart windows and façades within the general theme of technologies for improved indoor climate. His group studies fundamental and applied aspects of surface reactions on solid surfaces and photo-induced reactions on semiconducting materials with applications in indoor air cleaning, self-cleaning, and water cleaning. Recent internationally recognized results from his research include the invention of a simple method to modify acid-base properties of oxide surfaces based on photo-fixation of electrophilic or nucleophilic molecules from gas-phase (Handelsbanken Innovation Prize 2009; subject of commercialization), which also has been extended to a new low-temperature photocatalyst with superior sustained activity. His group has recently developed a new photocatalytic multilayer material for sustained indoor air-cleaning films for smart windows that allows for one-pass cleaning of VOC up to low ppm levels. Other recent activities include developed a new PVD methodology to prepare (001) facet-controlled anatase TiO2 nanoparticle films for photocatalysis applications; discovery of a general structure-reactivity relationship of photocatalytic anatase and rutile titania nanoparticles (patented); development of colloidal lithography for fabrication of ordered nano-patterned multi-layered photonic bandgap materials for photocatalysis applications, invention of microfabricated diamond IR waveguide methods for biomolecular imaging and integration with affinity layer technology (patented); and development of Raman imaging methods in nanomedical applications. Prof. Österlund has published 226 scientific publications including 6 invited book chapters, and he holds 6 international patents.

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Prof. Dr. Vladimir Ya. SHUR

School of Natural Sciences and Mathematics, Ural Federal University

Russia

Director of the Ural Center of Shared Use "Modern Nanotechnology", Ural Federal University, Ekaterinburg.
Professor of the Chair of Physics of the Condensed Matter and Nanosized Systems, School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg.
Head of Ferroelectrics Lab, School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg.
Honorary Worker of High Professional Education of Russian Federation, since 2005
IEEE Senior Member, 2016
Russian National Award Winner: "Professor of the Year" on Natural Sciences, 2018.
Author of more than 400 publications in peer-reviewed journals and 10 book chapters.
Hirsh Index – 33, number of citations – above 4000 (WoS).
He is the author of key results on nanodomain engineering in ferroelectrics. He is also known in the field of ferroelectric domain kinetics for elucidating works on the polarization switching.
He is currently engaged in research of the kinetics and statics of the domain structure in ferroelectrics, and micro- and nanodomain engineering in lithium niobate and lithium tantalate for nonlinear optical applications.

AWARDS:

Honorary Worker of High Professional Education of Russian Federation, since 2005
Russian National Award "Professor of the Year" on Natural Sciences, 2018.

PUBLICATIONS:

Papers: more than 400;
Joint monographs chapters 10;
Patents 10;
Citation index 4003; Hirsh index: 33 (Web of Science)

SUPERVISOR OF 23 PHD THESES.

RESEARCH INTERESTS:

- Domain engineering in lithium niobate and lithium tantalate for nonlinear optical application;
- Micro and nano-domain engineering in ferroelectrics;
- Ferroic domain structure: arising and evolution;
- Kinetics of phase transformations;
- Nanotechnology;
- Nanotoxicology;
- Material design and structural color inspired by biomimetic approach.

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Dr. Vladimir Shvartsman

Institute for Materials Science, University of Duisburg-Essen

Germany

PROFESSIONAL EDUCATION:

2015	Habilitation in Materials Science at University of Duisburg-Essen: "Investigation of polar structures in relaxor ferroelectrics by piezoresponse force microscopy" and a colloquium on: "Energy harvesting using the pyroelectric effect".
2000	Ph. D., Physical Chemistry, L.Ya. Karpov Institute of Physical Chemistry Moscow, Russia
1995	Graduated, Solid State Physics, Moscow Engineering Physical Institute, Russia, w. Distinction

RESEARCH AND PROFESSIONAL EXPERIENCE:

11/2009 – present	Lecturer and senior researcher at Faculty of Engineering, Institute for Material Science, University of Duisburg-Essen, Essen, Germany.
01/2005 – 10/2009	Researcher at Department of Physics, Applied Physics, University of Duisburg-Essen, Duisburg, Germany.
08/2001 – 12/2004	Postdoctoral researcher, Department of Ceramic and Glass Engineering, University of Aveiro, Aveiro, Portugal
06/1995 – 07/2001	PhD student, junior researcher, researcher at the Laboratory of Oxide Materials, L.Ya. Karpov Institute of Physical Chemistry, Moscow, Russia

RESEARCH INTERESTS:

- Study of functional materials with ferroelectric, piezoelectric, and electrocaloric properties.
- Investigation of nanoscale properties of functional materials using scanning probe microscopy techniques.
- Investigations of multiferroic materials: study of coupling between polar and magnetic subsystems (magnetoelectric effect); search for new types of magnetoelectric materials.
- Synthesis and characterization of composite functional materials.

SIGNIFICANT AWARDS AND HONORS:

Gottschalk-Diederich-Baedeker-Preis-2016 for the best Habilitation in the natural and engineering sciences at the University of Duisburg-Essen in 2015.

PROFESSIONAL ACTIVITIES

Reviewer for various scientific journals including "Nature Materials", "Physical Review Letters", "Physical Review B", "Applied Physics Letters", "Journal of Applied Physics", "Ferroelectrics", "Journal of the European Ceramics Society", "Journal of Physics D: Applied Physics", "Smart Materials and Structures

INVITED PRESENTATIONS

18 invited talks at international scientific conferences

Cumulative Total Number of Articles Published in Peer Reviewed Journals:
More than 140 papers in peer reviewed journals, three book chapters. H-index=31, number of total citations > 3300

Postgraduate students supervised
Total number of PhD students supervised/co-supervised, 5

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Prof. Aivaras Kareiva

Institute of Chemistry, Vilnius University of Latvia

Lithuania

Prof. Aivaras Kareiva is expert in the preparation and characterization of superconducting, optical and bioceramic materials bulk and thin films. He has published over 310 research articles in high level international journals. His Hirsch Index is 24. His articles were cited 2497 times. A. Kareiva visited many foreign universities (Helsinki University of Technology, Stockholm University, Harvard University, Rice University, Hasselt University, University of Saarland, University of Tuebingen, Masaryk University Brno, Tallinn University of Technology, University of Malta, Muenster University of Applied Sciences, Research Centre for Natural Sciences, Hungarian Academy of Sciences, University of Bern, Clausthal University of Technology, University of Cologne, University of Maribor, University of Geneva, Kyushu University, University of Venice, University of Strasbourg, Georgetown University and others). He supervised successfully 27 PhD students at Vilnius University, several postdocs and many foreign trainees. A. Kareiva participated or conducted several Research projects on optics and lasers with funding from NATO, the National Grant from Lithuania, the European Sixth Framework Programme, COST Action and Horizon 2020.

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Prof. JŪRAS BANYS

President of the Lithuanian Academy of Sciences
Professor at Vilnius University, Faculty of Physics
Lithuania

Jūras Banys graduated from Vilnius University in 1985, obtained PhD in 1990 and the second degree (doctor habilitatus) in 2000. Between 1988 and 1989, he was at Oxford University, UK, as a PhD student under the supervision of Prof. A. M. Glazer. He was awarded Humboldt Research Fellowship for post-doctoral scholars and spent the period of 1993–1995 at Leipzig University, Germany.

J. Banys published over 300 scientific papers. Currently his research group has been working on Relaxor Ferroelectrics and multiferoic materials. These investigations include single crystals, ceramics, thin films.

J. Banys won the Lithuanian National Prize for Science in 2002. In 2000 received P. Brazdžiūnas Award of the Lithuanian Academy of Sciences in the field of Experimental Physics. He is a member of the Lithuanian Physical Society, a member of the Lithuanian Materials Research Society, Member of the Lithuanian Academy of Sciences, Foreign member of the Latvian Academy of Sciences, Correspondent Member of the Saxonian Academy of Sciences in Leipzig,
member of the international advisory board of ECAPD (European Conference on Applications of Polar Dielectrics), member of the international advisory board of EMF (European Meeting on Ferroelectrics), member of the international advisory board of IMF (International Meeting on Ferroelectrics).

J. Banys has contributed to numerous Lithuanian national and international conferences as a Chair and Organizing or Program Committee Member.

e-mail: salak@ua.pt

Dr. Andrei Salak
Department of Materials and Ceramics Engineering and CICECO – Aveiro Institute of Materials, University of Aveiro
Portugal

Andrei Salak completed of his PhD in 1994 at the Institute of Solid State and Semiconductor Physics (Minsk, Belarus). In 2002, he received a post-doctoral position in CICECO - Centre for Research in Ceramics and Composite Materials at the University of Aveiro (Aveiro, Portugal). At present, A. Salak is an Invited Researcher at CICECO. He specializes in crystal structure determination and dielectric characterization of inorganic solids, particularly perovskite-like materials and layered ion exchangers. A. Salak is a co-author of more than 100 papers in international peer-reviewed journals with over 1000 citations and 1 patent. He has completed the supervision of more than 10 Master students and 2 PhD students. A. Salak is the Principal Coordinator of the project ‘Tuneable multiferroics based on oxygen octahedral structures’ (TUMOCS, 2015-2018, grant 645660) that receives funding from the European Union’s Horizon 2020 programme MSCA-RISE. http://tumocs.web.ua.pt/. The project joints 7 academic organisations and 1 SME from 6 countries. Besides, A. Salak is a Local Coordinator of the project MULTISURF (MSCA-RISE, grant 645676). He is also a PI of the R&D project POCI-01-0145-FEDER-0166 funded by P2020 COMPETE and FCT-Portugal.

e-mail: jpflaum@physik.uni-wuerzburg.de

Prof. Dr. Jens Pflaum
Experimental Physics VI, Julius Maximilian University, Würzburg
Bavarian Center for Applied Energy Research (ZAE Bayern e.V.), Würzburg
Germany

Jens Pflaum studied physics at the Ruhr-University in Bochum, Germany, where he received his PhD in 1999 for his work on magnetic resonance studies on exchange coupled ferromagnetic thin films. As a post-doc fellow at Princeton University from 1999 until 2001 his research focus shifted to organic thin films and their electronic transport properties. Returning back to Stuttgart University, Germany, in 2001 he extended this work to molecular single crystals which can be considered reference systems for studying fundamental questions on charge carrier and exciton transport in narrow bandwidth semiconductors and, in particular, its interaction with lattice dynamics. In 2008 he received a professorship at the Institute of Experimental Physics VI at Julius Maximilian University in Würzburg, where since then he is addressing questions on energy research and novel applications of organic semiconductors. By the strong application driven research he was appointed group manager for 'Organic Photovoltaics and Electronics (OPE)' at the Bavarian Center for Applied Energy Research (ZAE Bayern e.V.) in 2008 and holds membership in various scientific committee boards, including that of the 'International Conference on Organic Electronics (ICOE)' or the 'International Conference of Photovoltaics'.

Jens Pflaum's scientific interests span a broad range of topics, including fundamental questions on electronic and optical excitations in organic semiconductors and their implementation in thin film devices, such as OLEDs, transistors or photovoltaics. Recently he extended his activities to molecular based quantum devices, demonstrating the first, electrically driven single photon source at room temperature, as well as to thermoelectric applications of low-dimensional organic conductors.

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Dr. Luciana Vieira
Fraunhofer Institute for Interfacial Engineering and Biotechnology
Germany

SHORT BIOGRAPHY

Dr. Luciana Vieira studied chemistry and obtained her MSc. in materials science at the University of Campinas (Brazil). From 2008 to 2014 she was involved in several academic and industrial projects on electrodeposition of metals from deep eutectic solvents, ionic liquids and aqueous electrolytes at CEST (Center for Electrochemical Surface Technology, Austria). She obtained her PhD in 2014 at the Technische Universität Graz (Austria), where she continued her research on metal electrodeposition as a postdoc fellow. In 2015 she conducted postdoctoral research at the University of Campinas (Brazil) investigating the spectroelectrochemical properties of oxide nanomaterials. Since 2016 she has been working on the development of new electrocatalysts for energy conversion and storage, including electrochemical CO2 reduction, at the institute branch BioCat of Fraunhofer IGB (Germany). Since 2018 she is coordinating the European project CO2EXIDE (co2exide-eu.e-p-c.de).

PUBLICATION IN JOURNALS

1. Silveira, J. V; **Vieira**, L.L.; Aguiar, A. L.; Freire, P.T.C, Mendes Filho, J; Alves, O.A. and Souza Filho, A. G. Temperature-dependent Raman spectroscopy study in MoO3 nanoribbons, *Spectrochimica Acta A* **193**, 47-53 (2018).
2. **Vieira**, L., Burt, J., Richardson, P.W., Schloffer, D., Fuchs, D., Bartlett, P., Reid, G. and Gollas, B; Tin, bismuth and tin-bismuth alloy electrodeposition from halometallate salts in deep eutectic solvents, *Chemistry Open* **6**, 393-401 (2017).
3. **Vieira**, L.; Schennach, R. and Gollas, B; The effect of the electrode material on the electrodeposition of zinc from deep eutectic solvents, *Electrochimica Acta* **197**, 344-352 (2016).
4. **Vieira**, L.; Schennach, R. and Gollas, B; PM-IRRAS of a glassy carbon/deep eutectic solvent interface, *Physical Chemistry Chemical Physics* **17**, 12870-12880 (2015).
5. **Vieira**, L.; Whitehead, A. and Gollas, B; Mechanistic studies of zinc electrodeposition from deep eutectic electrolytes, *Journal of The Electrochemical Society*, **161** (1) D7-D13 (2014).
6. **Vieira**, L.; Whitehead, A. and Gollas, B; Mechanistic studies of zinc electrodeposition from deep eutectic electrolytes, ECS Transactions, 50 (52) 83-94 (2013).
7. Silveira, J. V; **Vieira**, L.L.; Mendes Filho, J; Sampaio, A. J. C.; Alves, O.A. and Souza Filho, A. G. Temperature-dependent Raman spectroscopy study in MoO3 nanoribbons, *J. Raman Spectroscopy* **10,** 1407-1412 (2012).

ORAL PRESENTATIONS IN CONFERENCES

1. **Vieira**, L., Csepei; L., Gärtner; T., Sieber, V; Energy as a Renewable Resource for Synthesis, **speaker and organizer** at the Valorization of Renewable Resource Meeting, Campinas - Brazil, 09.03.2018.
2. **Vieira**, L., Gärtner; T., Csepei; L., Steffler; F., Sieber, V Elektrochemische Anwendung von neuen klassischen Katalysatoren, **invited talk** at Seminar und Anwendertreffen: Elektrochemie – Anwendungen in Forschung und Technik, Frankfurt - Germany, 27.03.2017.
3. **Vieira**, L., Gärtner; T., Csepei; L., Steffler; F., Sieber, V Renewable energy as the driving force towards electrocatalysis, invited talk at the 26th ATC Industrial Inorganic Chemistry –Materials and Processes, Frankfurt - Germany, 24.02.2017.
4. **Vieira** L.L., Fuchs D, Schennach R, Bayer B, Gollas B. The Carbon Electrode/Deep Eutectic Solvent Interface: Electrochemistry and Spectroelectrochemistry, 12th ISEAC Discussion Meet on Electrochemistry and its Applications, Mumbai, India, 7-8.12.2016.
5. Gollas, B, **Vieira**, L., Fuchs, D. and Schennach; R., Electrochemistry and Spectroelectrochemisry of Carbon Electrode/Deep Eutectic Solvent Interfaces, *The 67th Annual Meeting of the International Society of Electrochemistry,* The Hague-The Netherlands, 25.08.2016.

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Prof. Andrey Lipovskii

Peter the Great St. Petersburg Polytechnic University
St. Petersburg Academic University
Russia

EDUCATION:

1970-1976	Undergraduate studies at Leningrad Polytechnic
1978-1981	Post-graduate studies at Leningrad Polytechnic

DEGREES:

M.Sci. (Radiophysics) in 1976 from Leningrad Polytechnic
Ph.D. (Technical Sciences) in 1981 from Leningrad Polytechnic (PhD Thesis "Integrated optics information processing devices")
Dr.Sci. (Physics and Mathematics) in 1992 from Russian National Examination Committee (Dr.Sci. Thesis "Materials and technologies of nonlinear integrated optics")

POSITIONS:

Since 2012	Full Professor at St. Petersburg Academic University and part-time Professor at Peter the Great St. Petersburg Polytechnic University (Head of Dept. of Physics and Technology of Nanostructures)
2009-2012	Full Professor at St. Petersburg State Polytechnic University, Vice-Head of Solid State Physics Dept., Vice-Dean of Faculty of Physics and Technology, part-time Professor at St. Petersburg Academic University
1992 -2009	Full Professor at St. Petersburg State Polytechnic University, Vice-Head of Solid State Physics Dept.,
1987-1992	Researcher, Senior Researcher, Associated Professor at St. Petersburg Technical University (former Leningrad Polytechnic)
1985-1986	PostDoc at Royal Institute of Technology, Stockholm, Sweden
1981-1984	Junior Researcher at Leningrad Polytechnic
1976-1978	Engineer at Leningrad Polytechnic

VISITING POSITIONS:

Visiting Professorship: University of Bordeaux, France; Shanghai Inst. of Ceramics, China; Cornell University, USA; University de Santiago de Compostella, Spain; Swiss Federal Polytechnic, Lausanne.
Visiting Researcher: University of Tsukuba, Japan; University Paris VI, France; University of Limoges, France.

TEACHING:

Lecturing: Solid State Optics, Quantum Electronics, Optical Information Processing, Integrated Optics, Nonlinear Optics.
Supervisor of Master and PhD students, Scientific Adviser of Doctor of Science Fellows.

SCIENTIFIC PAPERS, CONFERENCE TALKS AND PATENTS:

~250 research papers, h-index 26 (Scopus); ~200 talks at conferences and workshops, 6 patents

RESEARCH INTERESTS:

Material Science, Physics of Glasses, Diffusion and Ion Exchange, Nanostructures, Plasmonics, Nonlinear Optics, Integrated Optics, Semiconductor Lasers.

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Prof. Mitch M.C. Chou

Department of Materials and Optoelectronic Science
National Sun Yat-sen University, Kaushiung
Taiwan, R.O.C.

EDUCATION

2000	Ph.D. School of Optics/(CREOL), University of Central Florida, Orlando, FL. USA

EXPERIENCE

	Vice president for Research and Development, National Sun Yat-sen University, Kaohsiung, Taiwan.
2009 - Current	Current: Technical consultant, Korea Atomic Energy Research Institute (KAERI).
2010 - Current	Current, Ad joint research fellow, National Synchrotron Radiation Research Center, Taiwan.
2000 - 2004	Material research scientist, Crystal Photonics Inc., Sanford, FL, USA.

AREAS OF EXPERTISE

Single crystal growth, condensed matter physics

BIOGRAPHY

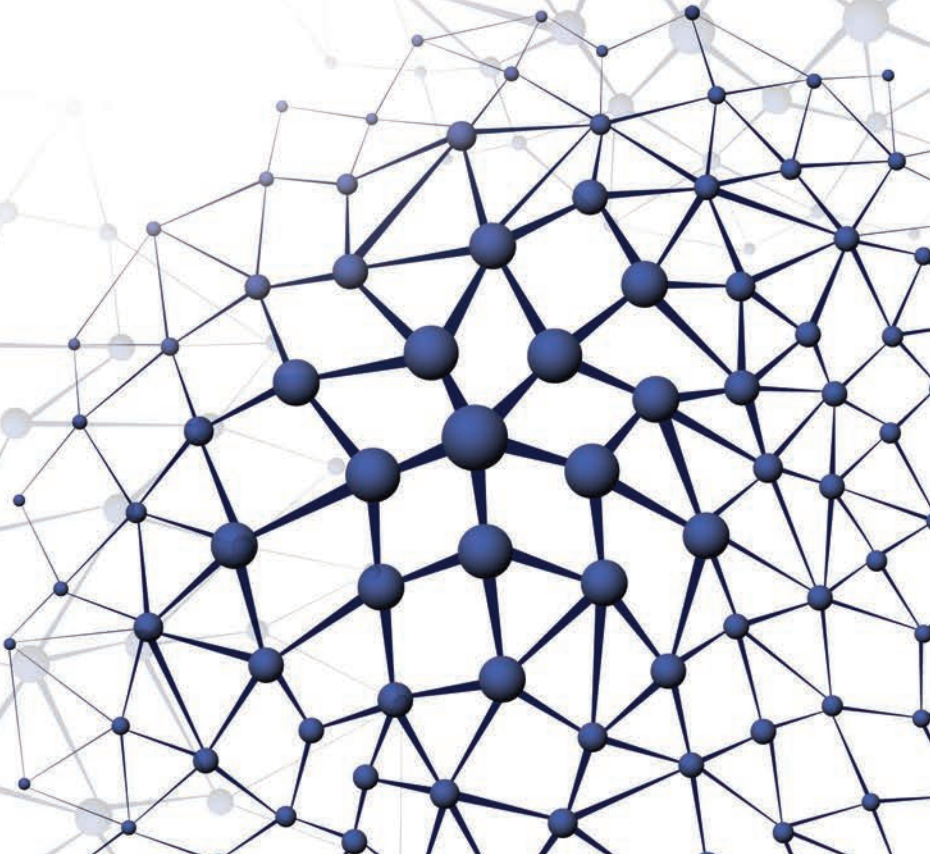
Professor Mitch Chou joined the faculty at NSYSU in 2004 and served as chair of the Department of Materials and Optoelectronic Science, 2012~2015. His current researches include laser, compound semiconductor, high temperature superconductor, topological insulator, and scintillator. He was a visiting scientist at some institutes in Germany, including Max Planck Institute for Solid State Research (MPI), Stuttgart; Institute of Applied Physics, Karlsruhe University; Institute of Crystal Growth (IKZ), Berlin; Paul Drude Institute (PDI), Berlin.

PROF. CHOU IS THE RECIPIENT OF

2014	Outstanding Scientific Contribution Award granted by Prime Minister of Taiwan
2012 & 2015	Outstanding Research Award of Ministry of Science and Technology (MOST), Taiwan

ABSTRACTS of the PLENARY PRESENTATIONS

International Conference Functional Materials and Nanotechnologies
‘FMNT – 2018’



PL-1

ESS and Its Contributions to Future Functional Materials and Nano Technology

Andreas Schreyer
European Spallation Source, P.O Box 176, SE-221 00 Lund, Sweden
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The European Spallation Source (ESS), which is currently under construction in Lund, Sweden, is designed to push the limits of research with neutrons to new horizons. ESS will open up new scientific opportunities which are complementary to those at X-ray sources. These will include unprecedented in-situ and in-operando experiments which are only possible with neutrons due to their special properties.

Fig.1 The Photo shows a recent view of the ESS construction site.

After a short summary of the design and the specifications of the European Spallation Source an overview of the current status and schedule of the ESS construction project will be given with a strong focus on the instruments and the surrounding scientific infrastructure. The overall goal of ESS is to begin user operation in 2023 and ramp up to 15 instruments by the end of 2026. Selected examples of new scientific opportunities in the field of functional materials and nano technology will be discussed.

PL-2

Material Science and Nanostructures Produced with GeV Heavy Ions

Christina Trautmann
GSI Helmholtzzentrum and Technische Universität Darmstadt, Germany
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The existing and future accelerator facilities at GSI and FAIR (an international Facility for Antiproton and Ion Research) provide unique opportunities for research with ion beams in many different disciplines [1]. The presentation gives a glimpse on the broad activities in the field of materials science and ion-track technology using swift heavy ions of GeV energy and above. The interest in such beams is based on the large energy deposition along the trajectory of each individual ion creating long nanoscopic trails of severe damage. In nanoscience, the small track size in combination with the large ion range (up to 100 µm and more) allows us to overcome limits of planar structuring techniques Several examples will be presented illustrating how to synthesize e.g. nanochannels and nanowires of tailored diameter, length, or shape with special electrical, optical, or thermal properties.

Ion beams at FAIR will permit materials science experiments with unprecedented ranges and intensities. Injecting for instance relativistic ions through a mm-thick diamond anvil of a high-pressure cell into a target under pressure, drives the local atomic structure far from equilibrium. Under such conditions, stabilization of new materials was evidenced via pathways in the phase diagram which are otherwise not accessible but of importance to simulate conditions existing in the Earth mantle. Testing materials behavior in extreme radiation, pressure, and temperature environments will also have a direct application to the understanding of structural materials degradation in next generation accelerator components, fusion and fission reactors, and shielding of equipment in deep space missions.

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PL-3

Nanoscale Piezoelectric Materials: Structure, Properties, Applications

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Recent studies revealed several new classes of piezoelectrics including 2D materials (graphene) [1] and biomolecular crystals (self-assembled peptides, amino acids, nucleotides) [2,3,4] Piezoelectricity in these occurs because of symmetry breaking on the surface in the first case and presence of highly anisotropic hydrogen bonds in the second. Graphene in contact with oxides offers extremely high piezoelectric activity due to polarity of C-O bonds, while peptide nanotubes (PNTs) demonstrate excellent electromechanical properties due to self-assembly and intrinsic softness of directed hydrogen bonds. Remarkably stable structure, possibility of functionalization together with biocompatibility and easy synthesis and nanofabrication, make graphene, PNTs and other biomolecular crystals (e.g. amino acid glycine [4]) attractive alternatives to traditional lead-based piezoelectrics.

In this presentation, the mechanisms of piezoelectric effect in these structures will be delineated and methods for their studies will be introduced. Hybrid Piezoresponse Force Microscopy (Hybrid-PFM) will be presented allowing nanoscale electromechanical measurements during acquisition of force-distance curves [6]. Several demonstrators including piezoelectric membranes based on 2D materials (graphene), cantilevers based on PNTs, and piezoelectric scaffolds for cardiomyocite cells [7] will be presented. Recent results on piezoelectricity and pyroelectricity in PNTs show that they are very attractive for various piezoelectric applications in biomedicine, because of their intrinsic biocompatibility combined with mesoporous structure and ability to work in contact with living cells and biological liquids. Scaling of piezomaterials down to nanosize is expected to dramatically improve their performance, thus making nanoscale piezoelectrics more sensitive than the traditional ones.

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PL-4

Making the Hospital a Safer Place by the Sonochemical Coating of the Textiles with Antibacterial Nanoparticles

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Sonochemistry is an excellent technique to coat nanomaterials on various substrates, imparting new properties to the substrates. After a short demonstration of coating NPs on ceramics and stainless steel, I'll present the coating of textiles such as polyester, cotton, and nylon. In all cases a homogeneous coating of NPs was achieved. Silver is known for generations as antibacterial, and indeed the Ag NPs have killed the gram-negative E. Coli (strain 1313) as well as the gram-positive Staphylococus aureus (strain 195) bacteria very efficiently. Lately, the FDA shows less enthusiasm towards nano Ag, as a result, we have moved to NPs of ZnO, and CuO as antibacterial agents. They were coated on the above-mentioned fabrics and showed excellent antibacterial properties. The coated textiles were examined for the changes in the mechanical strength of the fabric. A special attention was dedicated to the question whether the NPs are leaching off the fabric when washed repeatedly. The coated ZnO NPs on cotton underwent 65 washing cycles at 92 ^{0}C in water in a Hospital washing machine, no NPs were found in the washing solution and the antibacterial behavior was maintained. Recently, an experiment was conducted at PIGOROV Hospital in Sofia, Bulgaria in which one operation room was equipped with antibacterial textiles, namely, bed sheets, pajamas, pillow covers, and bed covers. 22 Patients in this operation room were probed for bacterial infections. Their infection level was compared with 17 control patient that were using regular textiles. The results are demonstrating that a lower infection level is observed for those patient exposed to the antibacterial textiles. Lately, we have synthesized NPs of a new material, $Cu_{0.89}Zn_{0.11}O$ that kills bacteria 10,000 times better than ZnO or CuO. The mechanism of the killing was studied and will be presented.

Coating of Catheters with the above mentioned NPs were performed and the coated catheters were inserted in rabbits. Results showed that the urine of the rabbits was not contaminated with bacteria and the growth of biofilm on the Catheters is avoided.

PL-5

Understanding Chemical Reactions Triggered by Defects on Energetic Materials and Interfaces. Insight from Quantum Chemistry

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Understanding, predicting, and controlling the materials response to external stimuli, such as heat, impact, spark, shock, and radiation continues to represent an outstanding challenge for both experimental and theoretical studies. Of a special interest are multifunctional materials and interfaces designed to achieve targeted properties. In this presentation, *ab initio* modeling of chemical reactions in solids will be highlighted. The role defects play in materials ranging from advanced perovskites to molecular crystals to energetic oxide interfaces will be discussed.

A stubborn challenge in the field of energetic materials (EM) is in gaining a reliable control over explosive chemistry. EM store large amounts of chemical energy, which can be rapidly transferred into thermal energy. The lack of understanding of microscale mechanisms of such a transfer leads to our inability to use an enormous potential of EM. We demonstrate that optical (laser) excitation of EM-metal oxide interface enables control of both the energy absorption and release. We show how surface defects (e.g., oxygen vacancies, F-centers) and charge transfer present new opportunities to ensure highly controllable photo-initiation of chemistry at the interfaces.

In the field of energy conversion, solid oxide fuel cells (SOFC) open the way of ecologically clean direct conversion of the chemical energy into electricity. However, the practical development of SOFC faces unresolved fundamental problems, in particular, concerning mechanisms of the electrode reactions. We illustrate how the crystal structure and morphology of materials (including defects and deformations) can be correlated with their stability mechanisms relevant to energy conversion and release. In particular, it will be revealed why $(Ba,Sr)(Co,Fe)O_3$ (BSCF) perovskites, which show the best cathode kinetics known for oxides, turned out to be unstable and hence lead to a reduced cathode performance under SOFC operating conditions, while $(La,Sr)(Co,Fe)O_3$ (LSCF) should offer a better alternative.

We recently applied the similar approach to understand interactions of toxic chemical warfare agents (CWAs) with existing filter materials. We explore various physical and chemical properties of CWAs including their reactivity in the gas phase, liquid solutions and interfaces to improve practical filtering systems.

PL-6

Advancing the Art Femtosecond Laser Writing

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Two decades ago it has been discovered that under certain irradiation conditions subwavelength structures with record small features of tens of nanometers, can be selforganized in the volume of fused quartz [1]. The negative optical anisotropy, which results from the alignment of nano-platelets, referred to as form birefringence, is of the same order of magnitude as positive birefringence in crystalline quartz.

Anisotropy of ultrafast laser writing also reveals in phenomena of quill writing and anisotropic photosensitivity associated with spatio-temporal couplings during ultrashort pulse propagation.

The control of light polatization allows direct writing elements of flat optics with spatially variant anisotropy, which exploits the geometrical or Pancharatnam-Berry phase shift.

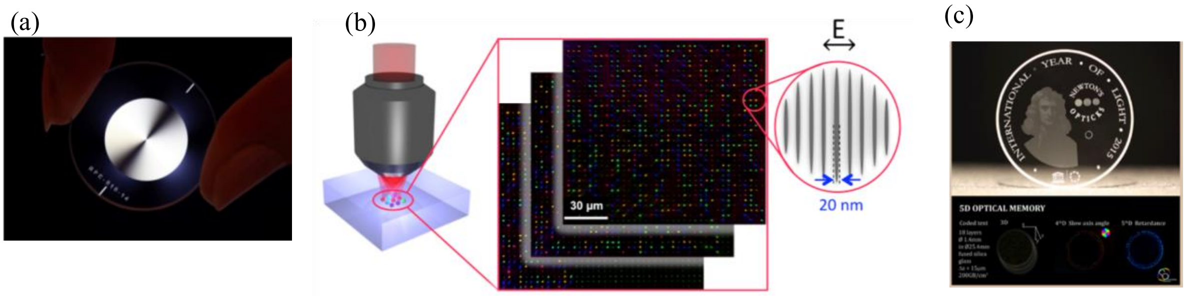

Fig. 1 (a) Femtosecond laser written S -waveplate in cross-polarized light; (b) 5 D optical storage ; (c) Eternal copy of Newton Opticks imprinted in glass.

The S-waveplate (Southampton-Super-Structured-waveplate) is one example of such birefringent optical element, which can be used for creating axially symmetric polarization state, e.g. radial or azimuthal, or optical vortexes with applications ranging from material processing to optical trapping (Fig. 1a).

The two independent parameters describing form birefringence in quartz glass, the slow axis orientation (4th dimension) and the strength of retardance (5th dimension), are also explored for the encoding of information in addition to three spatial coordinates (Fig. 1b). The storage allows unprecedented parameters including hundreds of terabytes per disc data capacity and thermal stability up to 1000°. The demonstrated recording of digital documents, which will survive the human race, is a vital step towards an eternal archive (Fig. 1c). The search of new material compositions for ultrafast laser nanostructuring is in progress.

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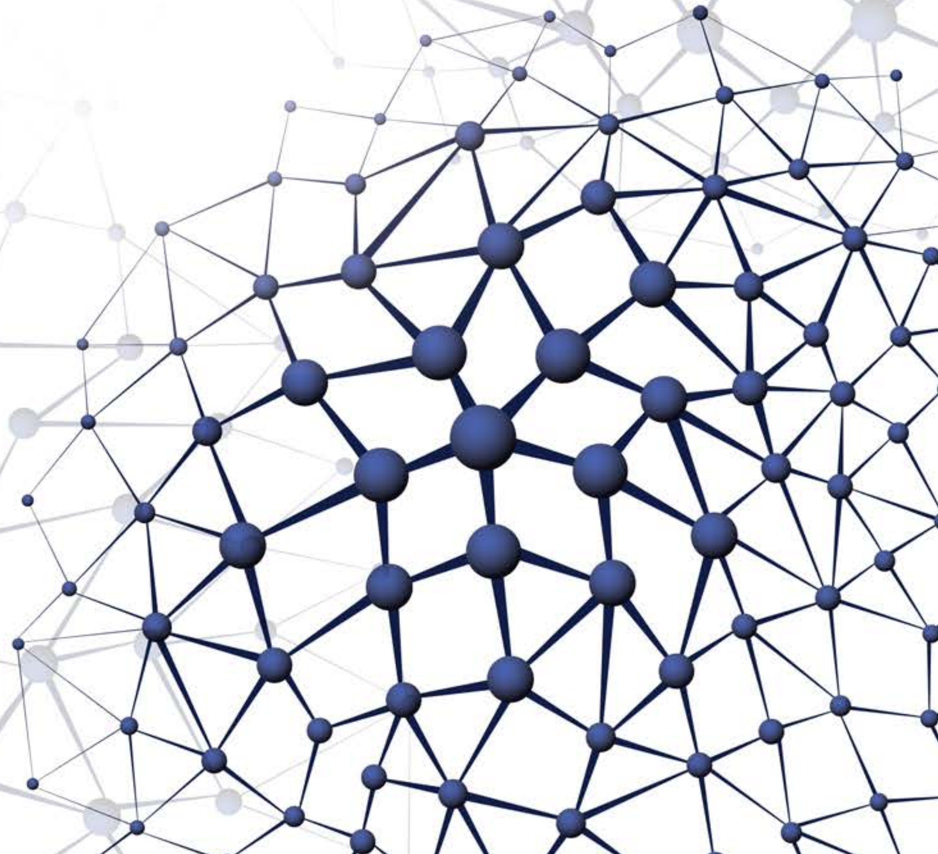
ABSTRACTS
of the INVITED PRESENTATIONS

International Conference Functional Materials and Nanotechnologies
'FMNT – 2018'



INV-1

MAX IV Laboratory in Lund, Sweden: Research Portfolio, Present Status and Expected Performance

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MAX IV Laboratory is a Swedish national laboratory providing bright x-ray beams for research in various fields. It operates two storage rings with 3 GeV and 1.5 GeV electron beam energy serving, correspondingly, hard and soft x-ray techniques. Additionally, the linear accelerator feeding the storage rings will also provide x-rays to the Short Pulse Facility for time resolved experiments.

The MAX IV 3 GeV storage ring is based on an original multibend achromat lattice for storing electron beam of ~300 pm·rad horizontal emittance. The generated x-ray beams have small linear and angular source size and thus high brightness and high degree of spatial coherence. These properties are essential for obtaining extreme focusing and enabling various innovative imaging and scattering techniques.

The MAX IV 1.5 GeV storage ring is based on a compact double-bend achromat lattice for the production of bright soft x-ray and UV radiation. This storage ring mainly serves beamlines with a variety of photoemission micro-spectroscopy techniques.

Presently, there are 16 beamline projects funded by either Swedish national funding agencies (Swedish Research Council (VR), VINNOVA, Knut and Alice Wallenberg Foundation, Swedish research universities) or international partners. These beamlines were proposed by the research community built around MAXlab – the predecessor laboratory operational in 1987–2015. Several beamlines have already entered the user operation, whereas others are in commissioning, assembly or design phase. The beamline portfolio is expected to grow up to around 30 beamlines in 2026.

In this talk, I present the unique properties of the MAX IV storage rings, consider various types of experimental x-ray techniques a) imaging, b) diffraction and scattering and c) spectroscopy, focus on a few research examples around the topics of the Conference: “nano materials”, “thin films” and “energy” and brief on the present status of the Laboratory. I also give some practical information on submitting beam time proposal, data policy and travel assistance.

INV-2

A Role of Large Scale Facilities in the Development of Novel Functional Materials

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Large scale research facilities, synchrotron radiation centres, have played a crucial role in fundamental discoveries and in the development of novel functional materials. This is thanks to advancing experimental methods based on superior radiation properties of storage ring based light sources. Namely, high brilliance of the radiation, specific time structure in ns-time domain and wide energy range from IR to hard X-rays are available for various experiments. In my talk, I will focus on the materials research carried out using time-resolved luminescence spectroscopy under VUV-XUV excitation at various research centres like DESY (Hamburg, Germany) [1] and MAX-IV Lab (Lund, Sweden) [2].

Synchrotron radiation has been an indispensable tool in the investigation of such short-wavelength emissions as cross-luminescence (CL) with ns decay and 5d-4f emission of rare earth ions [3]. Recent advances in band structure calculations, high demand on ultrafast scintillators for various applications and advancements of photodetectors (e.g., SiPM-s) with sensitivity shifted towards UV have renewed interest to such ultrafast emitters. Multication fluorides with complex band structure, e.g., K_2SiF_6, exhibit CL in UV-VUV and even visible regions as shown by us using pulsed cathodoluminescence. The studies at storage rings can provide a deep insight into the relevant processes challenging for ultrafast scintillation applications. A particular topic of the synchrotron studies of wide band gap nanomaterials is aimed at understanding the influence of nano-particle size and morphology on the fundamental electronic properties in comparison with bulk materials (see [4] for Al_2O_3). The peculiarities revealed via the excitation spectra of various intrinsic and extrinsic emissions in nano-alumina will be discussed. Finally, research challenges and experimental potential for luminescence spectroscopy at the FinEstBeAMS of the MAX IV Lab will be reviewed.

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INV-3

A Neural Network Approach for Structural Characterization of Metal Nanoparticles and Clusters

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Tracking the structure of heterogeneous catalysts under *operando* conditions remains a challenge due to the paucity of experimental techniques that can provide atomic-level information for catalytic metal species. Here we report on the use of X-ray absorption near edge structure (XANES) spectroscopy and artificial neural network for refining the three-dimensional geometry of metal catalysts. Neural network is used to unravel the *hidden* relationship between the XANES features and catalyst geometry. To train the neural network, we rely on the *ab-initio* XANES simulations by theoretical spectroscopy codes. Our approach allows one to solve the structure of a metal catalyst from its experimental XANES, as demonstrated here by reconstructing the average size, shape and morphology of well-defined mono- and bimetallic nanoparticles.[1] In the case of ultra-small clusters their average size can be estimated. This method is applicable to the determination of the structure of metal catalysts in *operando* studies and can be generalized to other nanoscale systems. It also allows "on-the-fly" XANES analysis, which is a required step for high-throughput and time-dependent studies, including the "reaction on demand" capabilities.

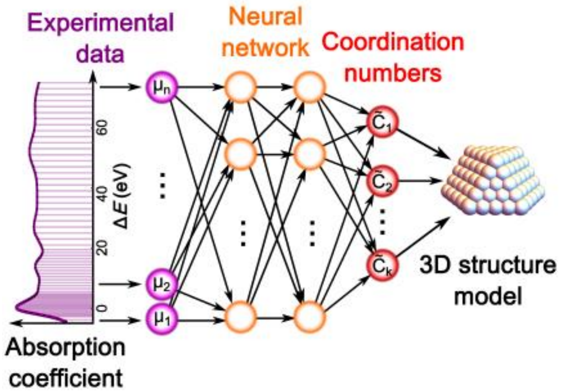

Figure 1. Illustration of the Machine Learning approach: feature space (absorption coefficient values) is mapped by neural network to nanoparticle-averaged coordination numbers that for well-defined particles can be interpreted in terms of specific sizes, shapes and structures.

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INV-4

Theoretical Modeling of Point Defects in Crystals

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Many practical applications of materials are based on the use of the properties caused by point defects, in particular those induced by radiation. Theoretical modeling of defective solids allows one not only explain existing experimental data but also predict the properties of new materials. For low defect concentration it becomes appropriate to model a single point defect in an environment of the remaining solid. In such a molecular cluster model the crystal with a single point defect can be seen as a gigantic molecule and the point defect properties are calculated using any of the methods of the molecular quantum chemistry. There are different possibilities to represent the rest of crystal: embedding into the crystalline environment (embedded cluster model), saturation by additional atoms (saturated-cluster model). However, in the case of a solid solution the single-defect model is not appropriate as the stoichiometry change is introduced by regular substitution of the host-crystal atoms by those of other chemical species. In this case the point-defect models with periodic boundary conditions (cyclic cluster and supercell) are more appropriate. These models allow one to use the computer codes and computational methods applied for both the perfect and defective crystals.

The symmetry aspects and applications of traditional supercell model of defective crystals are considered in [1, 2]. Recently a novel site symmetry approach for defective crystal calculations in the supercell model was suggested [3]. It is based on the group-theoretical analysis of the site symmetry of the split Wyckoff positions in the perfect crystal supercell, could be applied to a wide class of defects in crystalline solids and allows one to obtain more realistic values for the corresponding point defect formation energy. The efficiency of site symmetry approach was demonstrated for copper impurity in LiCl crystal [2], carbon-doped ZnO crystal [4], oxygen interstitials in corundum [5], polarons in cerium dioxide [6].

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INV-5

Photoluminescence Quantum Yield as a Test of Quantum Cutting Processes in Down-converting Phosphors

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Ionic-like down-converting phosphors nowadays are actively discussed for solar spectrum modification and in such a way for possible enhancement of the efficiency of silicon solar cells. Phosphors co-doped with Ce^{3+}–Yb^{3+}, Eu^{2+}–Yb^{3+} or Bi^{3+}–Yb^{3+} ions are of particular interest because of the efficient and broad absorption in UV-blue range and the near-IR emission around 1 μm from Yb^{3+}. However the real value of the energy transfer efficiency in such materials remains generally unknown. In other words, the question remains whether the energy transfer is cooperative (one-to-two) or non-cooperative (one-to-one energy transfer). This efficiency is usually estimated from shortening of the luminescence decay of donor (Ce^{3+}, Eu^{2+} or Bi^{3+}) ion, when the conversion ratio of 2.0 (*i.e.* an ideal quantum cutting mechanism) is postulated.

Instead of this we propose a direct measurement of quantum yield (QY), which allows to estimate a real value of the conversion ratio. This procedure was already tested by us for such phosphors as $Y_4Al_2O_9$ (YAM):Bi,Yb; Gd_2O_3:Bi,Yb; YVO_4:Bi,Yb; $YNbO_4$:Bi,Yb; $Y_3Al_5O_{12}$ (YAG):Bi,Yb; $Gd_3Ga_5O_{12}$ (GGG):Bi,Yb and YAG:Ce,Yb. Results for these materials will be presented and discussed. Our results testify that not all the phosphors that demonstrate the energy transfer from Ce^{3+} or Bi^{3+} to Yb^{3+} have the cooperative energy transfer. The procedure used in this study can be also applied to other systems proposed for quantum cutting in order to evaluate their performance for solar spectrum modification.

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INV-6

New Features of Hot Intraband Luminescence

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Intraband luminescence (IBL) is an ultrafast emission connected with the radiative transitions of hot electrons or holes between the sub-levels of the conduction or valence band of a crystal, respectively [1]. The spectrum of IBL is continuous, covering the whole transparency region of a material and growing in intensity towards NIR [2]. The characteristic decay time of IBL has not yet been accurately determined, but it is expected to be of the order of ~1 ps, reflecting the time scale of electron-phonon relaxation within the electronic bands. Despite IBL was discovered long ago, it has not been intensely studied mainly because of its very low intensity (estimated scintillation yield 20 photons/MeV [3]) and, correspondingly, unclear application perspectives. Recently, more attention has been drawn to ultrafast emissions due to increasing demands of medical and high-energy physics applications for higher scintillation time resolution [4].

Here we present a review of recent experimental and theoretical studies of IBL in various binary and complex wide-gap materials. IBL is observed typically under high-energy electron pulse (100-300 keV) excitation. We have shown that a direct observation of IBL is possible also under excitation by a low-energy (10 keV) continuous electron beam, pulsed X-rays and white-beam (3-60 keV) synchrotron radiation. The low-power excitation confirms the absence of an energy threshold for IBL creation. Excitation by X-rays allows predicting that the IBL can be excited by single photons of 511-keV energy, which makes it promising for enhancing scintillation time resolution in time-of-flight positron emission tomography (TOF-PET) [4], as IBL can provide an almost instant time marker for the event despite its low yield. The impact of various material features such as electron-phonon interaction and electronic band structure on the IBL spectrum shape and light yield will be analyzed.

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INV-7

Theoretical Modeling in Nanophotonics

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Several books have been published recently on various aspects of nanophotonics [1–4], and one of them [4] is fully devoted to organic nanophotonics. However, as strange as it may seem, molecular aspects of organic nanophotonics are almost not considered in [1–4]. Consequently, such important problems as molecules and molecular complexes, their structure, light absorption and emission, intermolecular charge and energy transfer in disordered organic functional layers, and calculations of the corresponding parameters remained outside the scope of [1–4]. This lecture is specially devoted to theoretical and computational aspects of these problems. Some of them were briefly considered in [5]. However, the main focus in [5] was on the simulation of nanophotonics structures. On the contrary, this lecture is devoted to modern quantum-chemical methods specially designed recently and currently used in the calculations of parameters required for the best description of excited states in organic molecules and in their intermolecular complexes (exciplexes), which are often characterized by significant intra- and intermolecular charge transfer. The set of these parameters include geometrical (structural) parameters and energy data for ground and excited states, charge and energy transfer parameters, light absorption and emission characteristics, and related properties.

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INV-8

Crystals for Optical Quantum Memory

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The title of my talk is the same as the title of our joint Project with Taiwanese colleagues, supported by the Russian Foundation for Basic Research (RFBR) from the Russian part and by the Ministry of Science and Technology (MOST), Taiwan. Mitch M.-C. Chou is Taiwanese Principal Investigator, he is responsible for the crystal growth and characterization by different X-ray and microscopy methods. I am Russian Principal Investigator and in addition to my group, two groups from Kazan' are involved into the Project. Gilman Shakurov from Zavoisky Physical-Technical Institute characterizes the crystals by EPR methods but the group of Sergei Moiseev carries out photon-echo experiments and measures coherence times of hyperfine levels selected to build a three-level Λ system for optical quantum memory.

In my talk, I'll briefly discuss the following points:

- Quantum informatics: quantum bits (qubits), quantum memory, quantum computer;
- Three-level Λ and V systems for optical quantum memory;
- Λ systems based on hyperfine levels of impurity centers in crystals;
- Requirements for crystals for optical quantum memory;
- A list of promising crystals;
- Several examples of our research [1-3].

Support by the Russian Foundation for Basic Research (Grant No 18-52-52001) is acknowledged.

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INV-9

Application of X-ray Microscopy in Materials Science and Nanotechnology

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X-ray imaging and X-ray computed tomography (XCT) provide non-destructive characterization capabilities on opaque objects, observing features with sizes spanning from millimeters to micrometers down to several 10 nanometers. Currently, two types of laboratory-based XCT setups are available commercially for imaging at medium and high resolution: micro XCT in projection geometry with a resolution of about 1 μm and nano XCT with focusing X-ray lenses with a resolution down to about 100 nm [1]. X-ray microscopy and nano XCT are potential techniques for nondestructive imaging of bulk materials and complex thin film structures. Examples for high-resolution X-ray imaging studies will be shown: reliability studies of microchips, kinetic reactions for energy storage and crack propagation in composites.

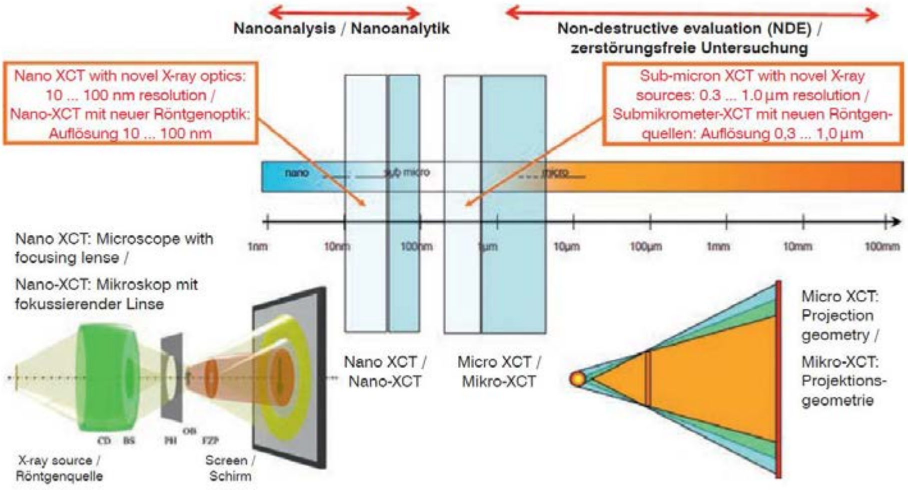

Fig.1 Imaging schemes for micro XCT and nano XCT and resolution ranges, today and expected future developments (3-5 years) [1].

Novel focusing lenses, so-called multilayer Laue lenses, have the potential to bring hard X-ray microscopy (high photon energy) to resolutions down to the 10 nm range and below, since - compared to the fabrication of state-of-the-art Fresnel zone plates - the resolution is not limited by the patterning process [2].

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INV-10

Novel Multi-functional Self-cleaning, Air Cleaning and Thermochromic Films for the Built Environment

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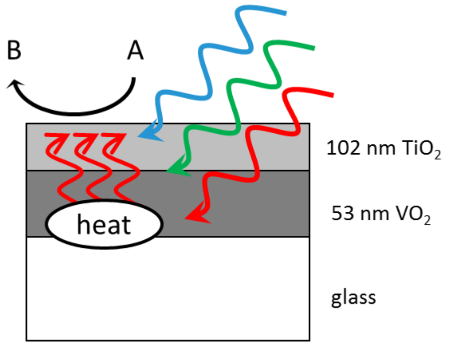

Fig.1 Principle of a spectral selective TiO_2/VO_2 multilayer coating on glass with enhanced (i) catalytic activity, (ii) thermochromic and (iii) anti-refelctive properties.

Spectrally selective photocatalytic multilayer films that exhibit dramatically enhanced photochemical reactivity upon solar light activation were fabricated. It is shown that synergistically enhanced physciochemcial properties can be achieved the surpass those of the constituting single-layer films. We present two case studies: TiO_2/VO_2 and TiO_2/TiAlN bilayer films made by reactive dc magnetron sputtering. The TiO_2/VO_2 bilayer exhibits enhanced near-infrared light absorption, which thereby heats the TiO_2 film by more than 15 degrees, resulting in an almost 2-fold increase of the reaction rate for photo-degradation of stearic acid layers. In addition, the TiO_2/VO_2 bilayer stack exhibited anti-reflective properties, and enhanced solar modulation (~ 9%) compared to VO_2, and ~ 20% increased solar absorptance compared to TiO_2. In the second example, bilayer TiO_2/TiAlN films yielded an almost 10-fold enhancement of the quantum yield for acetaldehyde removal (on par with state-of-the-art, heterojunction photocatalysts), and an associated temperature rise larger than 120 degrees. Both findings can be understood by thermal activation to the increase the surface reaction kinetics, where water desorption from the oxide plays and important role. We generalize the results, and discuss their implications for green building technology and possible scenarios for their implementation.

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INV-11

Shapes of Isolated Domains in Uniaxial Ferroelectrics

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The variety of domains shapes appeared in uniaxial ferroelectrics will be presented, classified and discussed using kinetic approach based on analogy between domain structure evolution and phase growth during first-order phase transformation. Recent investigations allowed revealing metastable domain shapes stabilized by bulk screening, which can be divided into: (i) circular shapes, (ii) regular polygons, (iii) irregular polygons, (iv) irregular shapes. The domain growth by step generation and kink motion has been discussed [1] with nucleation probabilities defined by local value of the sum of external field and residual depolarization field. This knowledge is applied for micro- and nano-domain engineering.

The complication of domain shape due to ineffective screening was demonstrated experimentally and by computer simulation [1]. Step nucleation variants have been considered: (a) stochastic - with equiprobable position of nucleation sites, (b) determined - with step generation at polygon vertexes and anisotropic kink motion. Stochastic nucleation creates circular domains, whereas determined nucleation - regular polygons. The convex polygons with oriented walls appeared for effective screening: (a) hexagons and triangles for C_{3v} symmetry ($LiNbO_3$ and $LiTaO_3$), (b) squares for C_4 ($Sr_xBa_{1-x}Nb_2O_6$), (c) rectangles for C_2 ($KTiOPO_4$) [2]. Screening retardation allowed formation of stars and irregular polygons [3]. The fast restoration of the initial domain shapes after merging was attributed to observed formation of the super-mobile walls [4]. The stochastic nucleation at elevated temperatures stimulates formation of fractal and dendrite shapes [5,6] created by: (i) discrete switching with subsequent merging, (ii) domain shrinkage, (iii) artificial dielectric layers [7].

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INV-12

Electrocaloric Effect in Barium Titanate Based Ceramics and Single Crystals

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Last years the electrocaloric effect (ECE), that is an adiabatic change of temperature of a dielectric material under an applied (removed) electric field, has attracted a significant attention opening possibilities for developing compact solid-state environmentally-friendly cooling devices [1]. Of particular interest are materials showing large ECE close to room temperature. Among them are solid solutions based on $BaTiO_3$. In these environmentally friendly compounds substitution in either A- or B-site of perovskite lattice allows to tune the ferroelectric-paraelectric phase transition, where the maximal ECE occurs. In spite of intensive studies, there is still a lack of direct measurements of the ECE.

We performed direct measurements of the ECE in $BaTiO_3$ single crystals [1], $Ba(Ti_{1-x}Sn_x)O_3$ (BTSn) [2], and $Ba(Ti_{1-x}Zr_x)O_3$ (BTZr) ceramics using both a modified differential scanning calorimeter and a specially built quasi-adiabatic calorimeter. In the single crystals we investigated anisotropy of the ECE. We showed that the value of the ECE depends on the direction of the applied electric field. Moreover, for the orthorhombic-tetragonal phase transition the electric field applied along $[001]_c$ direction results in the inverse ECE [1].

For the BTSn and BTZr ceramics substitution of Ti by Sn or Zr results in a merger of different ferroelectric phases of parent $BaTiO_3$ at $x \sim 0.10$. The corresponding compositions show the largest ECE. On further reducing of the Ti content a cross-over to relaxor behavior occurs. On the one hand, it is accompanied by decreasing of the maximal ECE value. On the other hand, the peak of the ECE broadens and a large ECE is observed in a broad temperature range. Results of the direct measurements are compared with the indirect estimation of the ECE from temperature dependences of polarization. The discrepancy between the results of the two methods is discussed.

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INV-13

Multicomponent Metal Oxide Systems for Optical and Magnetic Applications

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The phosphors host materials have proven to be of great importance for the optical function. Transition metal and rare-earth element ions have demonstrated lasing action in a wide variety of host crystals. Among the compounds which can incorporate transition metals or lanthanides several multicomponent metal oxide systems were elaborated [1-3]. Rare-earth aluminium garnets have also attracted considerable attention as host crystals for near-infrared solid-state lasers as well as for optoelectronics devices, including computer memories, microwave optical elements and as laser active media with applications in medical surgery and optical communications.

In recent years magnetic materials have been in the focus of interest, with much attention paid to their potential usage in modern technologies. Magnetic disks are used to read and write information, hard disk drives are used for storage of information. Iron containing garnets, perovskites and spinels with non-equivalent and antiferromagnetically coupled spin sublattices represent important classes of soft magnetic materials [4, 5]. The ferrimagnetic rare earth iron garnets, $R_3Fe_5O_{12}$, are unique group of materials, which have been long studied for their novel magnetic and magneto-optical properties.

The main aim of this study was to prepare different multifunctional mixed-metal oxides and investigate their suitability for usage as optical and magnetic materials.

Acknowledgements. The work has been done in frame of the project TransFerr. This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No. 778070.

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INV-14

Dielectric Response of the Methylammonium Lead Halide Solar Cell Absorbers

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Hybrid organic–inorganic perovskites have recently attracted overwhelming attention due to their excellent photovoltaic performance yielding efficiencies well exceeding 20%. This has been related to properties such as long charge carrier lifetime, the exceptionally large diffusion length, large absorption coefficient, high carrier mobilities, large open-circuit voltages, and direct band gap. The organo-lead trihalide perovskite compounds, $CH_3NH_3PbX_3$, are the forerunners in efficiency.

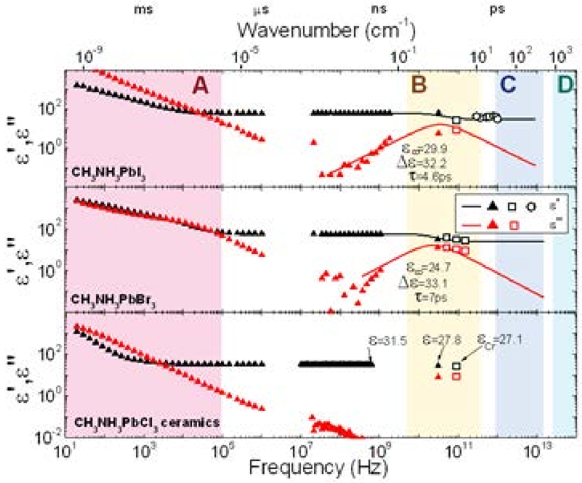

Fig.1 Frequency dependence of dielectric constant at room temperature for $MAPbX_3$ crystals.

In this presentation dielectric and acoustic properties in wide temperature and broad frequency range of organic – inorganic perovskites $CH_3NH_3PbX_3$ ($X = I$, Br, Cl) will be shown. Figure 1 shows dielectric constant of the three MA – Pb – halides across wide frequency range at room temperature. Sections denote the dominant micromechanism contributing to dielectric response:

A) Ionic motion/Dirft,
B) MA –dipole relaxation,
C) Anionic lattice dynamics (phonons),
D) Internal vibration of the MA molecule.

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INV-15

Tuneable Magnetic Co(II)-Containing Layered Double Hydroxides

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Layered Double Hydroxides (LDHs) are composed of the alternating positively-charged mixed metal M^{II}-M^{III} hydroxide layers and interlayers occupied by anions and crystal water molecules. The metal cations in the layers are coordinated by six oxygen atoms forming 2-D structures of the edge-linked oxygen octahedra. Anions of different nature (either inorganic or organic), size, configuration and charge can be intercalated into the interlayer. As a result, the characteristic layer-interlayer scale in LDHs can be from about 0.7 nm to several nanometers.

Our recent study revealed unusual magnetic behavior of some Co(II)-Al LDHs, particularly an anomalous temperature dependence of their effective magnetic moments [1].

Here we report on the systematic study of magnetic properties of Co(II)-containing LDHs. Layered double hydroxides with the Co(II)/Al cation ratio = 2, 3, and 4 intercalated with different anions were prepared and investigated. Magnetic characteristics and optical spectra of these LDHs were measured and correlated to the cationic composition and the interlayer distance. Magnetic susceptibility was calculated as a function of temperature for different cation ratios and possible distortions of oxygen octahedra. We show that the magnetic characteristics can be reversibly tuned by variation of the interlayer distance through anion exchanges and control of the crystal water content. The obtained LDHs are examples of tuneable nanomagnets and considered as promising models to study magnetic interactions in 2-D systems.

This work was supported by project TUMOCS – Tuneable Multiferroics based on Oxygen Octahedral Structures. This project has received funding from European Union Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 645660.

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INV-16

Low-Dimensional Organic Conductors for Thermoelectric Applications

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The intriguing properties of low-dimensional organic conductors distinguish them as interesting candidates for thermoelectric applications. In particular, their anisotropic metallic-like electrical conductivity reaching values of up to 10^5 S/m at room temperature in combination with a poor thermal transport characteristic for weak van-der-Waals bound crystals favor figures of merit, $zT = (\sigma S^2/\kappa)T$, that are of technological relevance. By the correlated electron system and its strong coupling to the surrounding lattice remarkable phenomena emerge, like phonon drag effects or the violation of the Wiedemann-Franz law, which support the implementation of organic conductors in future thermoelectrics even further [1].

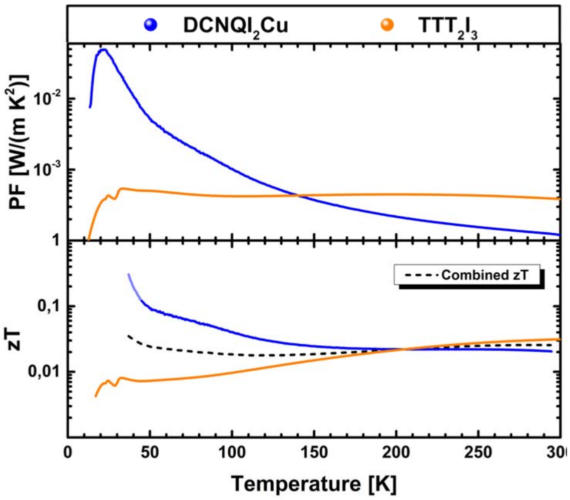

Fig.1 Temperature dependent power factor of n- and p-type conducting $DCNQI_2Cu$ and TTT_2I_3 radical ion salt crystals, respectively, (upper graph) and the related figures of merit (lower graph). From [2].

After introductory remarks on low-dimensional organic conductors and their correlated structural and electronic properties, we will demonstrate by means of two representatives of this class, the n-conducting $DCNQI_2Cu$ radical ion salt and the one-dimensional p-conductor TTT_2I_3, the complex thermoelectric behavior as function of temperature (see Fig. 1) [2]. Based on this information and the interdependence of the relevant quantities an all-organic thermoelectric generator comprised of the two organic conductors will be presented as a *proof-of-concept* and compared in its performance with alternative approaches. Strategies to further improve the thermoelectric performance of these low-dimensional organic conductors and their technological potential will be highlighted.

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INV-17

Functional Materials for the CO_2 –based Electrosynthesis of Ethylene Oxide

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The CO_2EXIDE project aims at the development of a combined electrochemical-chemical technology for the simultaneous electrocatalytic conversion of CO_2 to ethylene at the cathode, water oxidation to hydrogen peroxide at the anode and a subsequent chemical conversion of both intermediates to ethylene oxide and oligo-/polyethylene glycol in a cascade reaction. Within the project duration, the final CO_2EXIDE technology will undergo a thorough material and component R&D programme. A 1kW PEM electrolyser for CO_2-reduction and water oxidation in combination with an ethylene enrichment unit and subsequent chemical conversion cascade reactor will be manufactured to produce ethylene oxide as intermediate for oligo-/polyethylene glycol synthesis.

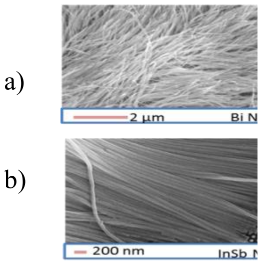

Figure 1: Possible range of nanostructures which can be obtained via different electrodeposition techniques at the Academic Centre for Materials and Nanotechnology, Kraków, with alumina templates: a) metallic bismuth (upper picture) or b) Indium-Antimony (lower picture).

For example, by using template-assisted electrodeposition it is possible to obtain hexagonally arranged nanowire arrays with huge active surface for electrocatalysis. Using e.g. 55 nm pore diameter alumina templates with 1 cm^2 geometrical area to obtain 200 nm long nanowires it is possible to get material with estimated 1357 m^2 active lateral surface. This can be easily improved by increasing the length of nanowires by introducing different shapes (periodically modulated or Y-branched) or by producing binary nanowires and etched on of components to obtain porous nanostructures. Examples of nanostructures obtained via template-assisted electrodeposition are presented in Figure 1.

Within the presentation, a detailed description of the CO_2EXIDE project and the materials development for nanomaterials as well as 3D-electrodes will be presented.

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INV-18

Plasmonic Nanoislands on Glass: Formation and Properties

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Optical properties of metal nanoparticles arise from their localized surface-plasmon resonances (LSPRs). These resonances give rise to strongly enhanced local fields near the metal-dielectric interfaces, which are advantageous for, e.g., catalytic activity, optical absorption and emission, as well as for Raman scattering and other nonlinear optical phenomena. We performed the studies of silver and gold nanoisland films (NFs) and isolated nanoislands (INs), including the structures covered with dielectric layers of different thickness.

The silver NFs and INs were formed on the surface of glass substrates subjected to silver-sodium ion exchange via out-diffusion of silver atoms reduced in hydrogen processing of the samples. In the case of the INs, thermal poling of the ion-exchanged glasses with structured anodic electrodes before silver reduction allowed the growth of one, two or several INs in the prescribed positions. Depending on the processing mode, nanoislands from 10-15 nm up to 200 nm in diameter were grown. The theory of the nanoislands growth was constructed. The gold NFs were formed from gold films deposited on the surface of glasses in the course of their self-arrangement under a thermal treatment. Atomic layer deposition (ALD) technique was used to cover the NFs and INs with dielectric TiO_2 layers. Linear optical properties of the metal core - dielectric shell nanoislands and virgin metal nanoislands were analytically and numerically modeled.

After the characterization of the size, morphology and LSPRs, the NFs and INs were tried in microRaman and the second harmonic generation (SHG) studies. The NFs and INs showed their applicability in Surface Enhanced Raman Scattering (SERS), with the efficiency comparable with one of commercial SERS substrates. Additionally, the NFs demonstrated a high temporal stability, and the INs allowed for high locality of SERS measurements. In nonlinear optical experiments, it was found that the TiO_2 cover provided ~50 times increase in the SHG efficiency [1]. A theory explaining this phenomenon was developed.

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INV-19

Epitaxial Growth of Cuprous Oxide by Molecular Beam Epitaxy and Electrodeposition

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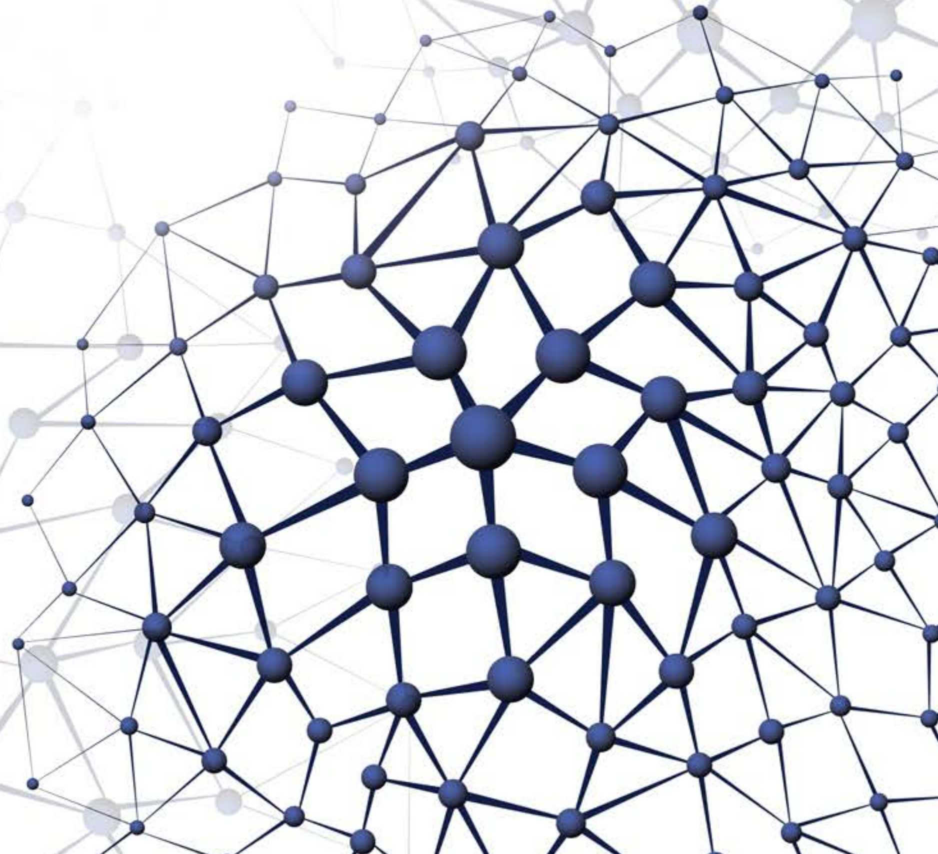
Cuprous oxide (Cu_2O) is promising material as a p-type semiconductor for solar energy applications. However, the performances of solar cells and thin film transistors based on Cu_2O are mostly inferior to expectation up to now. The reason responsible for the poor performance of the Cu_2O-based devices may be the fine-grained microstructure in which abundant grain boundaries act as recombination centers for electrons and holes. As a result, fabricating devices made from high quality Cu_2O epitaxial layer shall elucidate the reason. Various methods have been used to grow Cu_2O epilayers including molecular beam epitaxy (MBE), chemical vapor deposition and electrochemical deposition. In this study, studies on epitaxial growth of cuprous oxide on copper by MBE and on copper and silver by electrodeposition were carried out using an ex-situ method to study the orientation dependence of epitaxial growth. In this method, the substrates were polycrystalline and the substrate grain orientation was characterized by electron backscatter diffraction (EBSD) technique prior to deposition. The orientation distribution of the deposited films in the prior-analyzed area was characterized again after deposition by EBSD to reveal the orientation relationship between each deposit/substrate pair. Results indicated that Cu_2O preferred to grow epitaxially on {110} and {111} oriented grains with a cube-on-cube orientation relationship by MBE. Moreover, Cu_2O can be grown epitaxially on all silver grains by electrodeposition with the same orientation relationship. For copper substrates, an additional orientation relationship of <100>/45° was found between some epilayers and the underlying grains. Room temperature photoluminescence spectra showed that the epilayers grown by electrodeposition exhibited a strong near-band emission at approximately 1.95 eV.

ABSTRACTS
of the ORAL PRESENTATIONS

International Conference Functional Materials and Nanotechnologies
‘FMNT – 2018’



OR-1

Temperature Dependent Local Atomic Structure Studies of Bulk and Nanocrystalline CuO Using X-ray Absorption Spectroscopy

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Copper monoxide (CuO) is a prototype compound for high-T_c superconducting (HTSC) cuprates and is well suited to study the charge ordering phenomenon and compressibility of copper-oxygen bonds, which are crucial for the understanding of structure-property relationships in HTSC materials [1]. Electron-phonon and spin-lattice interactions play an important role in bulk CuO, which has monoclinic structure composed of CuO_6 octahedra strongly distorted by the Jahn-Teller effect. In particular, high-resolution XRD measurements [2] from 100 to 1000 K revealed anomalies in the lattice constants, appearing at the known antiferromagnetic phase transitions due to strong spin-lattice coupling. It was found recently [3] that small CuO nanocrystals with a size of ~5 nm experience giant negative thermal expansion (NTE) below the magnetic ordering temperature (~200 K), in spite of their thermal expansion at high temperatures is almost equivalent to that of the bulk CuO. The latter fact was used by the authors in [3] to rule out the lattice softening as the origin of the NTE and to explain the giant NTE by the magnetostriction effect being significantly enhanced in the CuO nanocrystals. Note that this conclusion is based solely on the unit cell parameters variation with temperature [3].

In this study, we investigate the change of the local atomic structure in nanocrystalline CuO in terms of a variation of both interatomic distances and atomic vibrational amplitudes. To our knowledge, such study has been never performed until now, but the EXAFS method is capable to address this problem [4].

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OR-2

Studies of non-crystalline Metal-organic Ligand Complexes Using Methodology Based on XAFS

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Metal-organic ligand complexes are being widely investigated due to fact that they in many cases exhibit higher biological activity and lower toxicity in comparison to free ligand. Among reports about the activity of complexes there is still insufficient information concerning metal-organic ligand binding mechanism. In particular it concerns complexes which were not obtained in a crystalline form. Structural information about them in such a case are rather speculated than experimentally determined. Inapplicability of diffration techniques causes that such compounds are not so widely studied.

In order to resolve molecular structure of the metal-organic ligand complexes in the non-crystalline state we have developed the methodology which is a combination of XAFS, elemental analysis, infrared and electronic spectroscopies (FT-IR, UV-VIS) and theoretical calculations performed at DFT level. Our methodology has been successfully applied to describe molecular structure of various bioactive Cu(II) complexes with hydroxycoumarins derivatives [1-3]. The microbiological activity for some of the studied complexes are comparable with commercially available drugs.

During presentation detailed information about methodology itself and results obtained for recently studied Ag(I) complexes with coumarin acids derivatives will be presented.

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OR-3

New Functional Material for Semiconductor Devices Protection against Electron Radiation

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Heavy elements are usually used as materials that effectively absorb high-energy radiation. The most often and widely used is lead, but it is a toxic material with a high density and a low melting point value. Uses of bismuth offer a very attractive alternative to lead protection from ionizing radiation due to the much more environmentally friendly Bi and its mass-dimension characteristics [1,2]. Samples of Bi coatings with 300-2580 μm thickness were electrodeposited from an acid perchlorate electrolyte. Samples radiation using a linear electron accelerator ELA-4 with 1.6-1.8 MeV energy was carried out. The shielding efficiency was evaluated by estimating the behavior of the volt-ampere characteristics of test p-MOS transistors (p-MOST). Bi coatings have a rhombohedral type of crystal lattice (space group R-3m) and fine-grained and dense structure (Fig. 1). The radiation-protection properties of Bi shields with electron irradiated p-MOST with an energy of 1.6-1.8 MeV and exposure doses up to 5×10^{14} cm^{-2} have shown that with reduced thickness d_{rth} values increasing from 1.0 to 2.6 g/cm^2, the value of the shielding efficiency K_a rises from 95 to 165. The most optimal, from the point of view of the mass-dimensional parameters, are $1.6 \div 2.0$ g/cm^2 d_{rth} values. Bismuth shields thickness increases to more than 2 g/cm^2 does not lead to a significant rising in K_a, which is due to braking radiation contributing to the shield absorbed dose.

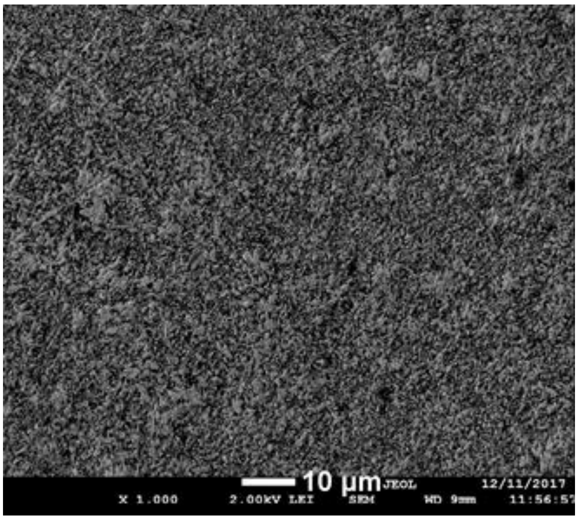

Fig.1 SEM image of Bi coating surface.

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OR-4

Understanding of the Kinetics of Defect Annealing in Heavily Irradiated Binary and Complex Oxides – Disordering Effects

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The binary and complex oxide (MgO, ZnO, BeO, Al_2O_3, $MgAl_2O_4$, $Y_3Al_5O_{12}$ etc) insulators as well as some other wide-band gap insulator and semiconductor compounds (AlN, BN, PLZT) are very important for many applications, including those when they are either exposed to radiation beams or function in radiation environment. This includes a huge number of applications, such as optical materials, phosphors, laser active elements, dosimeter, imaging plates, materials for fusion technology etc. The radiation-induced defects determine and affect functional characteristics of the corresponding devices and/or their specific elements. Thus, it is very important to predict/simulate not only the kinetics of diffusion-controlled defect accumulation under irradiation, but also a long-time defect structure evolution including the thermal annealing of radiation-induced defects.

After introducing some basics on the radiation point defects in halides, binary oxides and oxide perovskites [1] as well as the mechanisms of point defect formation under particle irradiation (neutron, ion, proton, electron), the current understanding of the point defect thermal annealing processes will be briefly reviewed.

We will present recent results and discuss current understanding of the kinetics of the *F*-type center annealing in above-mentioned compounds after electron, heavy ions or neutron irradiation, which were treated as the bimolecular process with equal concentrations of the complementary *F* and O_i defects. The process is controlled by the interstitial oxygen ion mobility, which is much higher than that of the *F* centers. The appropriate O_i migration energies were obtained from available in the literature experimental annealing kinetics for electron, neutron and ion irradiated MgO, Al_2O_3, $MgAl_2O_4$, $Y_3Al_5O_{12}$, BeO, ZnO, YSZ, PLZT etc. The results obtained are used for the evaluation of interstitial oxygen migration parameters and are compared with the available *ab initio* calculations.

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OR-5

Luminescence in Synthetic Hackmanites

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The natural hackmanite mineral $Na_8(AlSiO_4)_6(Cl,S)_2$ has been known for almost two hundred years for its photochromic properties [1]. The mineral changes color from white to pink under UV radiation [2]. Some natural hackmanites also have luminescent properties, usually exhibiting red luminescence under appropriate excitation [3]. Unlike natural hackmanites, synthetic hackmanites exhibit strong blue/white luminescence and persistent luminescence [4].

Luminescence in synthetic hackmanites originates from oxygen vacancies and titanium that is present as an impurity in the hackmanites [4]. The amount of titanium can also be increased in the sample by doping it in the synthesis process. This will increase the intensity of luminescence and persistent luminescence until a certain limit is reached. Replacing some of the Na in the sample with Li will also increase the luminescence intensity. The fact that the luminescence is achieved without lanthanides and the easy synthesis of hackmanites makes them an interesting option for luminescent materials used today.

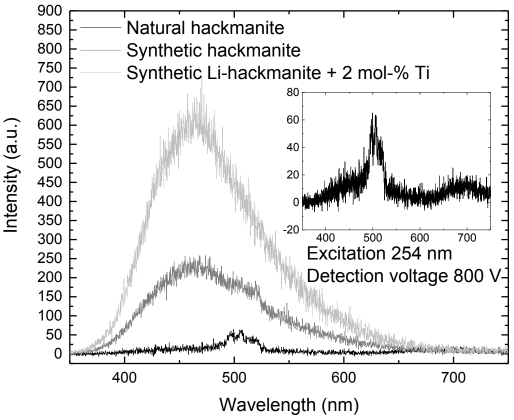

Fig.1 Luminescence in natural and synthetic hackmanites. The inset shows the zoomed spectrum for natural hackmanite.

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OR-6

280 nm Emission Band in $LiGaO_2$

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Lithium metagallate $LiGaO_2$ (LGO) is a wide band gap ($E_g \approx 6$ eV) oxide compound. Though up now it has found the main practical application as a substrate for semiconductor, its luminescence features are potentially promising for a more diverse application in optoelectronics. The samples examined are cut from a large crystal basically characterised by the producers in [1]. The luminescence spectrum contains several emission bands in the UV-visible light range, their features were described in [2]. The most interesting is the shortest wavelength emission band observed at 280 nm. Spectral location of the excitation spectrum of the 280 nm emission (entirely in the spectral range of fundamental absorption < 210 nm), its shape with a sharp peak around 205 nm, properties of the TL and afterglow creation spectra and photoconductivity's spectral response demonstrate that excitation corresponds to superposition of exciton and band-to-band transitions of $LiGaO_2$ crystal. Luminescence investigations including spectral, kinetic and polarization measurements in a broad temperature region, show that this band most probably has the complex nature combining emission from a bound exciton and tunnel recombination luminescence of donor-acceptor pairs with random distribution of separation distance. Studies of the polarised luminescence provide additional information about luminescence processes in $LiGaO_2$ crystal, confirming the complex nature of the emission and excitation spectra. Basing on results of the kinetics measurements and thermal behaviour of 280 nm band's intensity, which depends on excitation intensity and orientation of crystal and polarizer we suggest that peculiarities of the luminescence process are induced by the II order phase transition in LGO lattice.

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OR-7

Human Skin as an Optical Material

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Human skin can be regarded as a functional biomaterial, with a number of physiological functions – mechanical and biochemical protection of the internal organs, mechanical and thermal sensing, body thermoregulation, etc. Skin is also photosensitive, especially in the UVB spectral range; it is able not only to absorb light but also to emit fluorescent radiation. As a multi-layered structure, skin represents a nature material to be mimicked in functional materials and technical devices. Those and some other aspects make in-vivo skin an attractive objet to be studied by physical (e.g. mechanical, electrical,.magnetic and optical) methods. This presentation will focus on optical properties of skin that might be exploited in future developments of new functional materials and devices.

The main skin layers – stratum corneum, epidermis and dermis – are different from the point of optical properties. Specific optical parameters of each layer will be discussed, including refractive indices, spectral dependencies of absorption, scattering coefficients and anisotropy factors. Physical models of light propagation in skin will be regarded, as well. The main activities in the field of skin optics taken at Biophotonics laboratory of the Institute of Atomic Physics and Spectroscopy, University of Latvia will be briefly reviewed.

OR-8

Photocatalytic TiO_2 Thin Films for Air Cleaning Applications

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According to the World Health Organisation about 4.6 million people die each year from causes directly attributable to air pollution. The most common air pollutants are sulfur oxides, nitrogen oxides, carbon monoxide, VOCs, particulate matter, ammonia and radioactive pollutants.

One of the possible method to remove VOCs from outdoor and indoor air is photocatalytic oxidation. Generally, TiO_2 photocatalyst is used in two forms as a powder or immobilized form on a substrate. However, coatings prepared from nanopowders are less mechanically stable, i.e., have weaker adhesion to the substrate than thin films. Thus, the immobilization of TiO_2 with strong adhesion became a necessity for avoiding the release of nanoparticles into the environment.

In this study we show that transparent, smooth and well adhered TiO_2 thin films with a thickness of 200-300 nm can be used instead of nanopowders as photocatalytic air purification material.

TiO_2 films were deposited by the chemical spray pyrolysis method at various deposition temperatures in the range of 250 to 450 °C onto window glass and borosiliate glass and annealed at 500 °C. All films consisted of anatase TiO_2 with the mean crystallite size in the range of 20 to 35 nm. TiO_2 films on window glass show super-hydrophilic surface properties and sligtly lower photocatalytic activity than the TiO_2 film on borosilicate glass. The photocatalytic activity of TiO_2 on borosilicate glass was sufficient to fully decompose methyl-tert-buthyl-ether and acetone to CO_2 and H_2O.

OR-9

The Properties of Atomic Layer Deposited Zirconium and Cobalt Oxide Nanolaminates

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In connection with the demand for materials, which could be applied in the novel memories, ZrO_2 in nanocrystalline form could be a good candidate. ZrO_2 in stabilized cubic phase can exhibit enhanced ionic conduction, high dielectric permittivity and be magnetized nonlinearly in external fields [1]. Because of their possible advanced magnetic and electric properties, five-layer structures consisting of alternately deposited ZrO_2 and Co_3O_4 films were constructed in this study. The films were grown by atomic layer deposition at 300 °C from $ZrCl_4$, $Co(acac)_3$ and O_3.

All the films were crystallized in the as-deposited state. The multilayered structure was well-defined with interfaces between constituent, chemically and structurally distinct, layers (Fig 1). The dominant phase observed was the cubic ZrO_2 polymorph. The performance of the laminate films was dependent on the relative content of constituent oxide layers. The magnetization in these films was nonlinear, saturative, and with very weak coercive fields. Current-voltage measurements implied some tendency towards memristive behaviour with characteristic switching between lower and higher resistance states.

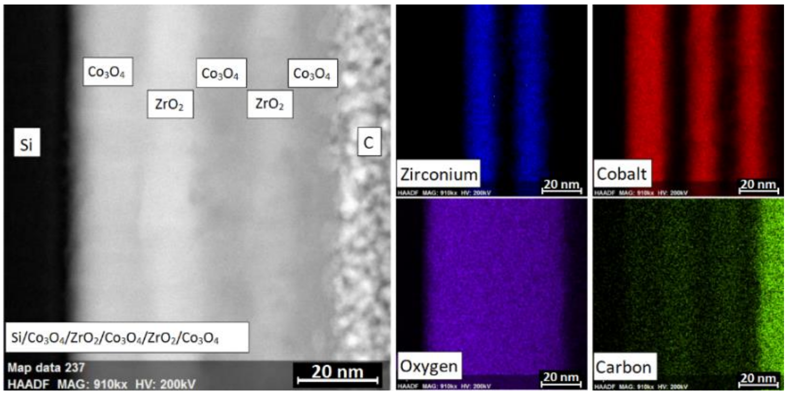

Figure 2. Cross-sectional EDX composition profiling of one of the ZrO_2-Co_3O_4 nanolaminates in the as-deposited state.

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OR-10

Thin Film Deposition by Magnetron Sputtering at Cryogenic Substrate Temperatures

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Magnetron sputtering is a well established tool for thin film deposition. Majority of work on sputter deposited films has been done either without intentional heating or cooling of the coated substrate or – mostly when highly crystalline films are to be deposited – with the substrate heated up to a few hundred degrees centigrade. Cooling is often used upon coating of plastic substrates, where it is done to avoid thermal damage to the substrate rather than to influence the properties of the growing film. Even if it has been demonstrated that at cryogenic temperatures the films grow differently [1], deposition at low temperatures is still a very scarcely studied field.

We report on a sputtering system with the substrate holder designed for cryogenic temperature deposition. The cooling is achieved by liquid Nitrogen circulation.

To provide an example of unique possibilities provided by the cryogenic temperatures, we focus on Zinc oxide film deposition. Zinc oxide based films are widely studied for a variety of applications [2], including transparent conducting oxides with *n*- and *p*-type conductivity. At room temperature, the sputter deposited films grow as wurtzite ZnO. For the films deposited at cryogenic substrate temperatures, Raman and IR spectroscopy studies show a peroxide structure pertinent to ZnO_2, which is a higher oxidation state than can be obtained at room temperature even under extremely Oxygen-rich deposition conditions. The wide vibration bands are indicative of amorphous or nanocrystalline structure. The studies are underway to examine the transformations the films may undergo upon exposure to higher temperatures in different atmospheres, as well as to find a suitable further treatment to obtain p-type conductivity.

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OR-11

Lead-free Ceramics on the Base of Sodium-Bismuth Titanate and Sodium-Potassium Niobate

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Influence of cation substitutions on stoichiometry, structure parameters, dielectric, ferroelectric, and piezoelectric properties of ceramics based on $(Na_{0..5}Bi_{0.5})TiO_3$ (NBT) and $(K_{0.5}Na_{0.5})NbO_3$ (KNN) perovskites was studied. The samples were characterized using the X-ray Diffraction, Scanning Electron Microscopy (SEM), Second Harmonic Generation (SHG), Dielectric Spectroscopy, and Atomic Force Microscopy in Piezorespone Force Microscopy mode (PFM) methods.

Ceramic samples in systems $(Na_{0.5}Bi_{0.5})TiO_3$ - $BaTiO_3$ (NBT-BT) and $(K_{0.5}Na_{0.5})NbO_3$ – $BaTiO_3$ (KNN-BT) additionally modified by Li^+, Mn^{3+}, Ni^{3+} and Fe^{3+} cations (1-5 mol.%) were prepared by the two-step solid-state reaction method at temperatures of 700 – 1400 K.

Ferroelectric phase transitions near ~ 400 K and ~ 550 K (NBT) and at ~700 K (KNN) were revealed in the dielectric permittivity versus temperature curves of ceramics studied. Remnant hysteresis loops were received for separate grains in the samples using switching spectroscopy PFM method. Local PFM hysteresis loops for the samples studied were observed indicating ferroelectric polarization switching at nanoscale. Increase in the spontaneous polarization value was proved for modified ceramics using the SHG method.

Non monotonous changes of the dielectric parameters ε_{rt}, $\tan\delta_{rt}$ and maximum effective local d_{33} values were observed in modified BNT- and KNN-based compositions confirming their prospects for new lead-free materials development.

Acknowledgment

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OR-12

Influence of Powder Milling Time on the Microstructure of the Lead-Free $K_{0.5}Bi_{0.5}TiO_3$ Ceramics

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Search for materials not containg lead in composition is one of the priorities of the environmental policy promoted by the European Union's. An expression of the actions carried out is the European Union's Directive - RoHS (limitation of hazardous substances in electrical and electronic equipment). The Directive specifies the maximum weight concentration of such elements in the composition as: Pb lead, Cd cadmium, mercury Hg and hexavalent chromium Cr^{6+}. The value of these composition should be 0.1% (0.01% for cadmium) [1].

Among many lead-free materials, one of the most prospective for replace lead-based compounds is potassium-bismuth titanium $K_{0.5}Bi_{0.5}TiO_3$ (hereinafter referred to as KBT). This material belongs to the group of compounds with a perovskite structure of general formula $A_{0.5}^{1+}Bi_{0.5}^{3+}B^{4+}O_3$. KBT in the room temperature has tetragonal symmetry and relatively high Curie temperature T_c=653 K [2]. Serious disadvantage of this compound, which is already visible at the technological level, is the low density of the samples [3].

The paper presents the influence of powders milling time on the KBT microstructure. Bismuth oxide Bi_2O_3 (SIGMA-ALDRICH, 99.9%), titanium oxide TiO_2 (SIGMA-ALDRICH, ≥ 99%, pure) and potassium carbonate K_2CO_3 (SIGMA-ALDRICH, 99.9%) were used as starting substrates. The milling time of the substrates was changed in the following sequence: 1, 2, 4, 8 and 12 hours. Sintering of the samples was carried out in two-stages. The apparent density were measured by the Archimedes method. The control of microstructure was performed by scanning electron microscopy (SEM).

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OR-13

Carrier Recombination and Diffusion in $MAPbI_3$ and $MAPbBr_3$ Perovskite Crystals in Wide Excitation Range

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Recently lead halide perovskite crystals have attracted much attention for application in solar cells, narrowband photodetectors [1], two-photon pumped lasers and autocorrelators [2], while detailed excitation dependent carrier transport properties were scarcely addressed. In this work $MAPbI_3$ and $MAPbBr_3$ crystals grown by inverse temperature crystallization method were studied. Light induced transient grating, time-resolved free carrier absorption and time-resolved photoluminescence methods were applied for investigation of excitation dependent carrier diffusion coefficient, lifetime and diffusion length in wide excitation range (see Fig. 1) complementing one- and two- photon excitation at 480-680 nm and 1053-900 nm wavelengths, respectively.

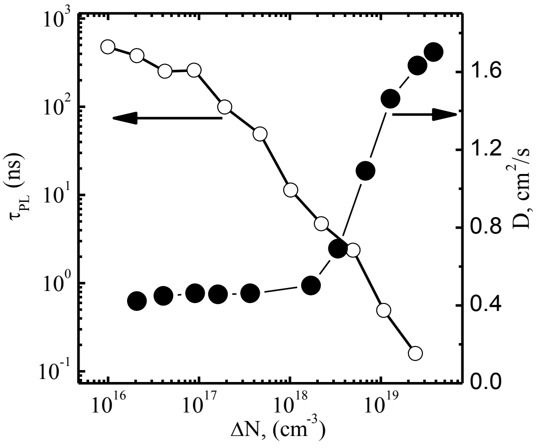

Fig.1 Photoluminescence decay time and diffusion coeficient excitation dependences in $MAPbBr_3$ crystal.

At low excitations 1-2 μs long lifetimes were observed due to nonradiative recombination on defects, while increase of excitation provided bimolecular and Auger recombination coefficients of 1, 4 $\times 10^{-10}$ cm^3/s and 1.5; 1.2×10^{-29} cm^6/s for $MAPbI_3$ and $MAPbBr_3$ crystals, respectively. At low excitations diffusion coefficient values of 1.35 cm^2/s and 0.45 cm^2/s were obtained in $MAPbI_3$ and $MAPbBr_3$, respectively. These values increased with excitation due to plasma degeneracy. Simultaneously determined lifetime and diffusion coefficient values provided excitation dependent diffusion length, reducing from 10 μm to 0.1 μm in $10^{16} – 4\times10^{19}$ cm^{-3} excess carrier density range.

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OR-14

Ab initio Calculations of ABO_3 Perovskite (001), (011) and (111) Surfaces, Interfaces and Defects Therein

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Ab initio calculations for main ABO_3 perovskite surfaces, namely $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $SrZrO_3$, $BaZrO_3$, $PbZrO_3$ and $CaZrO_3$, were performed [1-9]. For ABO_3 perovskite (001) surfaces, with a few exceptions, all atoms of the upper surface layer relax inwards, all atoms of the second surface layer relax outwards, and all third layer atoms, again, inwards. The relaxation of (001) surface metal atoms for ABO_3 perovskite upper two surface layers for both AO and BO_2-terminations, in most cases, are considerably larger than that of oxygen atoms, what leads to a considerable rumpling of the outermost plane. The ABO_3 perovskite (001) surface energies always are smaller than the (011) and especially (111) surface energies. The ABO_3 perovskite AO and BO_2-terminated (001) surface band gaps always are reduced with respect to the bulk values. The B-O chemical bond population in ABO_3 perovskite bulk always are smaller than near the (001) and especially (011) surfaces. Electronic and atomic structure of $BaTiO_3/SrTiO_3$ and $SrZrO_3/PbZrO_3$ (001) interfaces are analyzed [10]. Systematic trends of *F*-center calculations in ABO_3 perovskite bulk and on their (001) surfaces are analyzed [3,11].

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OR-15

Oxygen Diffusion in Ti-Al Alloys

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The development of new high temperature structural materials based on titanium aluminide, the mechanical properties of which will be between the properties of nickel-based superalloys and high-temperature ceramics, is a challenging problem of modern materials science. In this connection it is necessary to understand better the mechanism of surface oxidation of Ti-Al alloys at the microscopic level. This implies theoretical studies of the interaction of oxygen with a surface and its diffusion from surface into bulk and also in bulk alloys in dependence on their composition. In this work we discuss the oxygen diffusion properties in Ti_3Al, TiAl and $TiAl_3$.

The calculations were performed by the projector augmented wave method within density functional theory. It is shown that oxygen prefers to be adsorbed in the Ti-rich positions on the surface and in bulk. The absorption energies of oxygen increase with the titanium content in Ti-Al alloys. The preferential O diffusion paths were established for considered alloys. The barrier limiting O diffusion in the alloys corresponds to 0.25 eV in $TiAl_3$, 1.15 eV in TiAl and 2.42 eV in Ti_3Al. The temperature diffusion coefficient was calculated using statistical approach. Calculated results are found to be in a good agreement with experimental data [1] as seen in Fig. 1 for Ti_3Al. In general, the oxygen diffusivity decreases with increase of Ti content in the set $TiAl_3$-TiAl-Ti_3Al because Ti-rich sites can trap oxygen that retards its diffusion and hinders aluminum oxidation. The impurity influence on the key migration barriers is discussed.

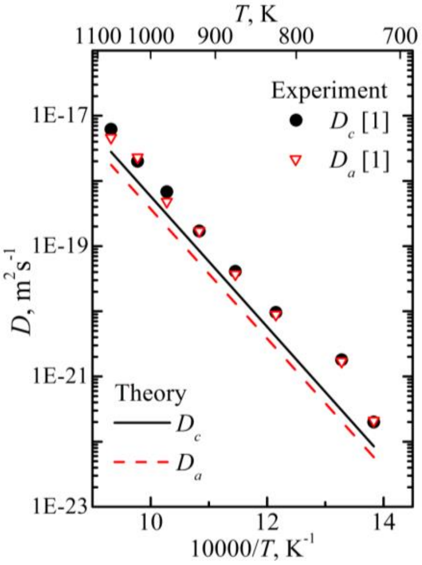

Fig. 1. Calculated and experimental diffusion coefficients of oxygen in Ti_3Al.

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OR-16

Electron Paramagnetic Resonance in Glass Ceramics

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Glass ceramics are composite materials, which consist of one or more crystalline phases embedded in a glass matrix. When doped with rare earth ions, these materials show promising optical properties for applications in phosphors, infrared radiation up-converters and optical temperature sensors. Luminescence of rare earth ions is strongly influenced by their local atomic surroundings, therefore, formation of defect centres must be controlled when designing novel materials.

The power of electron paramagnetic resonance (EPR) lies in its ability of characterizing the electronic structure and atomic arrangements at paramagnetic point defect sites very accurately. In glass ceramic investigations EPR spectra enable to identify, whether paramagnetic activators have incorporated the crystalline phase of the material as well as to determine their local structure.

In this report the applicability of EPR spectroscopy in glass ceramic investigations will be overviewed. The available literature data of transition metal (Mn, Cu, Cr) and rare earth (Gd, Eu, Er, Yb) element ion paramagnetic probes as well as our own recent results in oxyfluoride glass ceramic system investigations will be reviewed.

OR-17

Effect of Grain Size on Microstructure, Transformation Behavior and Functional Properties of Ti-Ni Shape Memory Alloy

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Shape memory alloy Ti-50.7 at.%Ni with various B2 austenite grain sizes (GS) from 5 to 15 μm was studied. The SEM observations were carried out using a JSM-6460LV. The microstructure was studied using a JEOL 2100 TEM. Characteristic temperatures were measured using a “Mettler Toledo” DSC. Energy dispersive spectroscopy (EDS) was carried out using the EDS stage of a JEOL 2100. Functional properties (FP) were studied using bending.

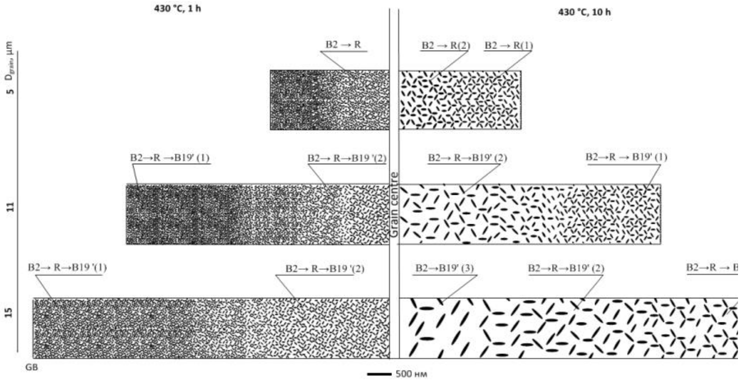

Fig.1 Schematic illustration of microstructures after solution treatments and aging. The bars represent a cutting from the grain.

The distribution of Ti_3Ni_4 phase particles is heterogeneous (Figure 1), the degree of which depends on the aging time. It is weak after aging for 1 h and becomes pronounced with increasing aging time to 3 and 10 h. The effect of annealing time on the temperature of the B2→R transformation is not pronounced. In the fine-grained structure (GS = 5 μm), B19′ martensitic formation is suppressed, and this does not depend on the aging time. The formation of B19′ martensite becomes possible with GS growth above 11 μm and an increase in the degree of heterogeneity of the microstructure, when particles of the Ti_3Ni_4 phase with a diameter greater than 70 nm precipitate in the GI. The appearance of a B2→B19′ transformation is observed in the structure with the largest GS of 15 μm at the maximum aging time. This is associated with the loss of the coherency between coarse Ti_3Ni_4 precipitates (~350 nm) and the matrix.

The maximum total recovery strain ~16% and recovery strain 15,5±0.5 alloy is provided by the structure with the GS 5 μm. Effect further aging at 430 ºC on FP is ambiguous and depends on the exposure time under aging and the GS. It is accompanied by their degradation in fine-grained alloy and improves them in the coarse-grained alloy.

OR-18

Features of Nanostructure and Functional Properties Formation in Ti-Ni SMA by ECAP Method Under Quasi-continuous Mode

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The effect of severe plastic deformation by equal-channel angular pressing (ECAP) under normal and quasi-continuous regimes on the structure and the mechanical and functional properties of a Ti–50.2 at % Ni shape-memory alloy (SMA) has been studied. ECAP was carried out at an intersection angle of channels of 120° using a regular regime with heatings between passes at 450°Cin 20 passes and a quasi-continuous regime at the temperature of 400°C in three, five, and seven passes. The hot screw rolling with subsequent annealing at 750°C for 30 min and water cooling was used as a reference treatment (RT).

Comparison of two different ECAP routess showes that for the most effective improvement of the functional properties of the Ti-Ni SMA, it is necessary to use ECAP (at $\varphi = 120$ °) in the quasi-continuous mode, since the ECAP with pauses and intermediate heatings is accompanied by considerable softening.

The optimum temperature range of the ECAP application (at $\varphi = 120$ °) in the quasi-continuous mode of 400-450 ° C was determined. Lowering the deformation temperature below 400 ° C is accompanied by the destruction of the billet.

As a result of the quasi-continuous ECAP at 400°C in 7 passes, a mixed nanocrystalline and nanosubgrained structure was obtained with an average size of the structure elements (grains/subgrains) of 103 ± 5 nm and a high density of free dislocations, ensuring a high level of a completely recoverable strain of up to 7.3% without post-deformation annealing, and up to 9.5% with annealing at a temperature of 400 ° C, 1 hour. The texture changes during the ECAP processing are estimated.

OR-19

Nematic Mesomorphous Systems Based on Dispersions of Carbon Nanotubes and Mineral Particles

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Fluid systems containing nanocarbon and/or mineral particles are in the focus of research interest due to a plethora of applications: nonlinear optical power limiting (OPL), photo-dynamic therapy, photo-conversion and electrical energy storage, sensors, etc. Relatively recent potential application of such systems would concern getting stable biaxial nematic phase, anticipated to have promising abilities in display technologies owing to the shortened response time of particles' medium axis with respect to the external field. Liquid crystals have been studied extensively during last decades and abundance of information has been collected. However, there is still a lot of gaps.

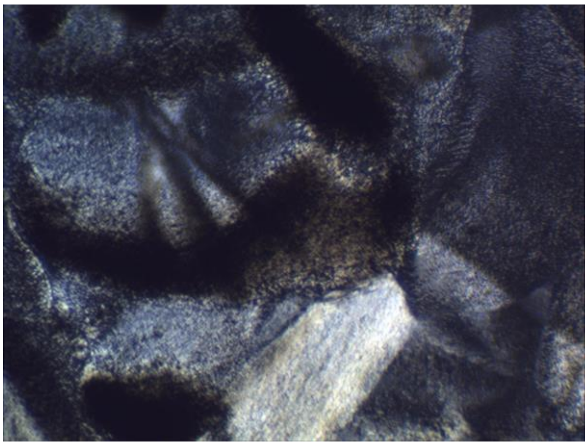
Fig.1 SWCNT-based mesophase in polarizing microscope.

We discuss a long-standing issue of getting a biaxial nematic phase, anticipated to demonstrate shorter response time of the system with respect to the 2nd director in the external field. We discuss stabilization of mineral rod+plate aqueous suspensions by an extremely elongated moieties with regard to decay into a blend of uniaxial nematics. In first place, we report on the statistical-thermodynamic description of the phase diagram in ternary mixtures of particles with D4h symmetry on the platform of the restricted-orientation Zwanzig model on the 3rd virial level. We also give an account of processing regular nematic suspensions of single wall carbon nanotubes (SWCNT) and mineral components (goethite) as pre-requisits of getting ternary suspensions with biaxial ordering.

OR-20

Influences of Sputtering Process Factors on Wear Resistance of TiN Coated on a Machine Component

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In this work, effects of sputtering process factors including DC current, pressure and Ar to N_2 flow rate ratio on wear resistance of TiN coated on cast stainless steel of a fishing net-weaving machine part namely, an upper hook were systematically investigated using 2^k factorial design, analysis of variance (ANOVA) and other statistical tools. Wear testing experiments of the TiN coated upper hooks were carried out on the real fishing net weaving machine. A normal probability of effects and main and interaction effect plots of process factors were constructed in order to identify the statistically significant process factors and to determine an appropriate operating condition of the process factors with the lowest weight loss. The Ar to N_2 flow rate ratio and the interaction between the pressure and the Ar to N_2 flow rate ratio were found to be statistically significant while pressure and sputtering DC current were not statistically important.

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OR-21

Determination of the Electron Effective Mass for n-type Germanium by the Low-frequency Impedance Dispersion

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The basic method of determining the effective mass of charge carriers in semiconductors is a cyclotron resonance method. Also there is work to define the effective electron mass via Faraday effect. In both cases the electric charge motion in a magnetic field are considered.

In this work we define the effective mass of the electron in the n-type germanium (doped with Sb in concentrations $10\cdot10^{14}$, $3.7\cdot10^{14}$, $2\cdot10^{14}$ and $0.8\cdot10^{14}$ cm^{-3}) by analyzing the low frequency dispersion of the complex impedance [1]. The spectrum was recorded by Frequency Response analyser PSM1735 NumetriQ.

Samples of 10×10×5 mm were measured in the crystallographic direction [111] (electrodes were pressed to surfaces of 10×10 mm).

The effective mass (m^*) was determined from the formula for the DC conductivity of the semiconductor [2]:

$$\sigma_o = \frac{e^2 n\tau}{m^*},$$

where e – electron charge, n – charge carrier (electron) density, $\tau = 1/\omega_\tau$, ω_τ – frequency, corresponding to the maximum in the complex impedance diagram $Z''(Z')$ (Fig.1). It is shown that the value of the effective mass electron in Ge depends on the carrier density (Table 1). Here m_e is the free electron mass.

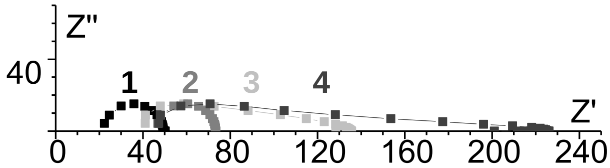

Fig.1 Complex impedance diagrams for Ge with n : $10\cdot10^{14}$ (1), $3.7\cdot10^{14}$ (2), $2\cdot10^{14}$ (3) and $0.8\cdot10^{14}$ (4) cm^{-3}.

Table 1. The results of calculating the effective mass of n-type germanium

n	$10\cdot10^{14}$ cm^{-3}	$3.7\cdot10^{14}$ cm^{-3}	$2\cdot10^{14}$ cm^{-3}	$0.8\cdot10^{14}$ cm^{-3}
$\rho=1/\sigma_0$	1.5 Ω·cm	4 Ω·cm	7.5 Ω·cm	20 Ω·cm
m^*	1.2 ± 0.2 m_e	0.9 ± 0.2 m_e	2.3 ± 0.4 m_e	3.4 ± 0.6 m_e

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OR-22

Ceria-based Electro-chemo-mechanical Actuator with Ti/$Ce_{1-x}Gd_xO_{2-x/2}$ Composite Contacts

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Chemo-mechanical effect of a solid refers to dimensional change due to change in stoichiometry. Dimensional change due to charged defects moving in an electric field has been termed the electro-chemo-mechanical (ECM) effect. Such instability is clearly deleterious for batteries or fuel cells, but, as recently suggested, has a potential for use in actuation. A typical ECM actuator scheme includes: electrode1\WB1\solid-electrolyte(SE)\WB2\electrode2, where WB denotes working-body solids with large chemical expansion coefficient. We have constructed a room temperature ECM nanocrystalline membrane actuator (2mm diameter; ≈2μm thick) with Gd-doped ceria as SE. We tested two alternatives for WB's: (1) metal/(metal oxide) or (2) ceria/metal nanocrystalline composite. Electrical and electromechanical measurements demonstrated that actuator response with metal/metal oxide WB is limited by the rate of oxygen diffusion from the solid electrolyte to the metal surface. Actuators with ceria/metal composite WB provide faster response time (≈20sec) and larger vertical displacement (>3.5μm).

OR-23

CAMART² – Regional Development Opportunity

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The CAMART² ('Excellence Centre of Advanced Material Research and Technology Transfer') project is aimed to upgrade the existing Centre of Excellence at the Institute of Solid State Physics, University of Latvia (ISSP UL), which was established in 2001 by the former project CAMART, realised within EC FP5. The CAMART² project is based on a long-term partnership between ISSP, KTH Royal Institute of Technology – the largest technical university in Sweden, and RISE – Research Institutes of Sweden. ISSP is renowned for its scientific achievements in applied materials physics for micro- and nanotechnology, electronics, photonics, functional coatings and related theoretical and characterization capability.

The vision of CAMART² is to establish ISSP UL as the most important centre of excellence for education, science, innovation and technology transfer in the Baltic States. ISSP UL will also become the hub for a collaboration and technology transfer platform called "RIX-STO", for materials physics including scientists, entrepreneurs, investors and policy makers on both sides of the Baltic Sea.

The active involvement of the Swedish partners assures successful modernization of ISSP UL, including an overall refinement of the educational programs, strengthening of the research and development activities towards higher technology readiness levels, establishment of an innovation system and Open Access Laboratories, as well as ISO 9001 certification.

The partners play a substantial role in an ambitious program for networking and outreach to make a real impact on academia and high-tech industries in the region around Riga and Stockholm, with respect to scientific results, economic growth and increased competitiveness. The region will benefit from injection of highly educated young people, closer collaboration between academia and industry, and offering state-of-the-art open access research infrastructure boosting innovation and economy.

OR-24

Solar Energy with New Generation Power Electronics Solutions

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In the frames of the Interreg project Green Power Electronics [1], financed by the European Regional Development Fund, we compare the efficiency of traditional Si based power electronics with efficiency of the new generation devices, where Si is replaced by GaN and SiC [2].

Fig.1 Physicum's solar-energy test station.

The demonstration pilot on smart houses (see Fig.1) aims to demonstrate the higher efficiency of advanced power electronics based inverters compared to traditional Si-based inverters [3]. The example of results obtained with three test systems, having 12 solar cells and one traditional inverter in each system, are presented in Fig.2. Figure shows the influence of solar panel direction (NE, SW or both together), depending on the time of the day. The solar irradiation and local temperature, measured by the weather station of the institute of physics, are presented on the same figure. Next generation inverter prototypes will be tested with two remaining test systems (Fig.1.) in summer 2018. The results of these tests are presented in poster session of FMNT-2018.

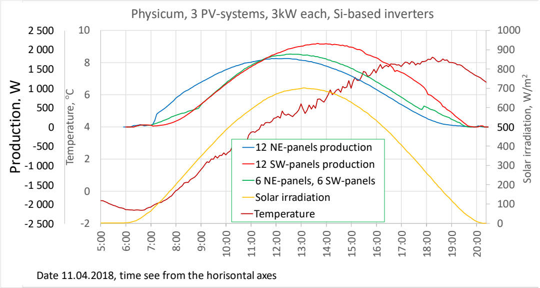

Fig.2 Example of the solar energy production using traditional Si-based inverters on the Physicum's test station in spring 2018.

At the present moment (spring 2018), the companies around the Baltic see don't offer the new generation materials based inverters at all. But they intend to do this in the near future. GreenPE project helps all interested companies with consultancy service, helping to implement modern power electronics solutions and reduce energy wasted for just heating the environment.

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OR-25

Baltic TRAM – a Network of Industrial Research Centers Providing Analytical Services for Business Innovation in the Baltic Sea Region

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The international consortium of the Baltic TRAM (Transnational Research Access in the Macro-region) project has created a network of Industrial Research Centers (IReCs), operating in all EU countries around the Baltic Sea 2016-2018 [1]. IReCs organize and provide services for businesses in order to enable access to analytical research capacities of academic and non-academic R&D institutions in the region. Such smart cross-border cooperation between IReCs opens new horizons for small and medium-sized enterprises in their product and service developments using top-level analytical equipment available in the countries of consortium members.

The main goals of the Baltic Tram are the following: establish an active IReC network and provide analytical services to 60 companies. For this purpose, the Baltic Tram consortium has built up communication channels between IReCs and with the target group - entrepreneurs, created databases of analytical resources in the Baltic Sea region, settled evaluation process of service applications by experts and further management of the service process (incl. contracting, feedback system, etc.). In our presentation we will demonstrate achievements of the Baltic Tram by showing the portfolio of services accommodated and research fields (industrial branches) addressed. Baltic Tram is contributing to the European open data policy by a pilot project, in the framework of which necessary regulations were formulated and an IT-environment was created, making data collected within Baltic Tram services available to interested parties. Various analysis and mapping of local policies (e.g., smart specialization) and practices (e.g., voucher schemes) have resulted in the policy recommendations and the concise Briefing Notes providing the regional overview, respectively. Challenges and efforts in creating a sustainable IReC network operating beyond the project duration in the Baltic Sea Region will be discussed.

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OR-26

Advanced Materials and Technologies in Fusion Research: An Overview and Some Recent Results from Latvian EUROfusion Laboratory

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The scientists of Institute of Solid State Physics, University of Latvia (ISSP UL) actively participate in the materials research on fusion. The Association EURATOM-University of Latvia was established in 2001 and ISSP UL became a coordinator of the Latvian Research Unit (since 2014 – Latvian EUROfusion Laboratory).

In this presentation, we briefly review the current Latvian activities in basic research at the national level, as well as participation at the international level, in cooperation with other institutions from the EUROfusion consortium.

Tasks included will be:

- Multiscale theory and modelling of functional materials for diagnostics;
- Kinetics of radiation defect creation and recombination;
- First principles large scale modelling of radiation defects and processes;
- Critical comparison of different types of irradiation (electrons, protons, neutrons, heavy swift ions);
- Peculiarities of diffusion-controlled recombination kinetics at high radiation fluencies;
- Comparison of radiation properties of single crystals and ceramics;
- Validation of computer modelling by advanced materials (including understanding the mechanism for nucleation of Y_2O_3 precipitate in the ferritic steel lattice (ODS));
- Radiation and thermally resistive materials.

Finally, some recent experimental and theoretical results of the completed/ongoing Latvian EUROfusion research projects, focusing on the exploration of radiation and heat-resistant materials practically used in fusion experiments, will be highlighted.

OR-27

Impedance Spectroscopy of Water Splitting Reactions on Nanostructured Metal-based Catalysts

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Hydrogen production by water splitting using nanomaterials as electrocatalysts is a promising route for replacement of fossil fuels by renewable energy sources. In particular, development of inexpensive non-noble metal-based catalysts is necessary in order to replace currently used expensive Pt-based catalysts on a large scale. Impedance spectroscopy is a versatile method to study the hydrogen and oxygen evolution reactions, thus laying the groundwork for an increased understanding of the connection between material properties and performance.

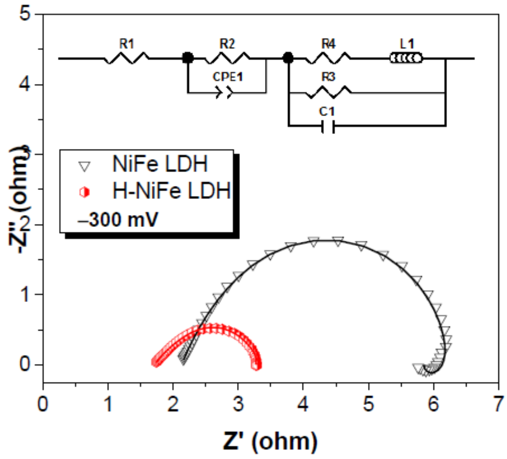

Fig.1 Nyquist plots for two NiFe-based catalysts at -300 mV overpotential versus RHE. The inset shows the equivalent circuit, where the right-hand part is one of the H-C models [1] and pertains to the hydrogen evolution reaction.

In this paper we report on a detailed impedance study of Ni-Mo and Ni-Fe based electrocatalytic materials deposited onto porous and compact substrates. The impedance parameters depend greatly on the morphology and character of the substrates. Results were interpreted within the framework of Harrington-Conway (H-C) [1] and double R-CPE [2] equivalent circuit models. Optimized Ni-Fe based catalyst showed very promising properties, yielding an electricity-to-fuel conversion efficiency of up to 83% at current densities of 10 mAcm-2. The materials were analyzed in terms of their frequency response during the water splitting reaction. Ni-Fe displayed an inductive impedance response at low frequencies, which is related to the presence of an adsorption step in the reaction.

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OR-28

First Principles Calculations of Perovskite Solid Solutions for Fuel Cells

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Two types of ABO_3-type perovskite solid solutions (BSCF: $Ba_{1-x}Sr_xCo_{1-y}Fe_yO_{3-\delta}$ and LSCF: $La_{1-x}Sr_xCo_{1-y}Fe_yO_{3-\delta}$), mixed ionic – electronic conductors, continue to attract attention because of a wide range of potential applications in modern technologies, e.g. gas separation membranes, solid oxide fuel cells (SOFC), etc [1,2]. The point defects, in particular oxygen vacancies are decisive for the transport properties and greatly affect the performance of perovskite materials in specific applications.

We present the results of first principles large scale computer calculations of defective BSCF and LSCF, and discuss the thermodynamic stability of the cubic phase under different conditions [3,4]. We explored and analyzed in great detail the oxygen vacancy formation energies in the cubic and hexagonal phases of BSCF and demonstrated that a high concentration of vacancies (oxygen non-stoichiometry), in fact, stabilizes the cubic phase over the hexagonal phase. We also discuss peculiarities of the oxygen vacancy diffusion in BSCF and LSCF. We observed a considerable charge transfer between the migrating oxygen ion and the adjacent *B*-site cation in the transition state of diffusion, which is the main reason for the exceptionally low oxygen migration barrier in BSCF [5]. The smaller size mismatch between *A*- and *B*-site cations in LSCF results in twice higher vacancy formation energy and higher migration activation barrier, which give rise to a smaller oxygen vacancy concentration and thus a slower oxygen exchange reaction, as compared to BSCF.

Based on the above-discussed results of first principles calculations of the defect formation and migration energies, as well as oxygen atom and molecule adsorption on perovskite surfaces, we calculated the kinetics of oxygen reduction reaction (ORR) at the surface as a function of adsorbed oxygen and surface vacancy concentrations [6]. This allowed us to determine *the rate-determining step* (which is important for improvement of fuel cell and permeation membrane performances) and suggest an interpretation of available experimental data. Special attention is paid to the role of polar surface termination on the ORR rate.

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OR-29

$LaNiO_3$-based Oxygen Electrodes for Solid Oxide Electrolysis Cells

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While K_2NiF_4-type $La_2NiO_{4+\delta}$ and its derivatives attract significant attention as prospective cathode materials for intermediate-temperature solid oxide fuel cells, a perovskite-like counterpart, $LaNiO_{3-\delta}$, has not been considered for these applications, mostly due to the limited phase stability under ambient oxygen pressures. On heating in air, it decomposes at ~1000°C; cathodic polarization can be expected to induce the decomposition of perovskite phase at even lower temperatures characteristic for IT-SOFC operation. On the contrary, redox changes imposed by anodic polarization under oxidizing conditions should not be of risk for the phase stability of $LaNiO_{3-\delta}$. The present work aimed to explore $LaNiO_{3-\delta}$ as potential oxygen electrode material for solid oxide electrolysis cells.

$LaNiO_{3-\delta}$ ceramic powder with rhombohedrally-distorted perovskite-like structure was prepared by glycine-nitrate combustion synthesis followed by calcinations in oxygen atmosphere at 800-1000°C. Porous $LaNiO_{3-\delta}$ samples (sintered in O_2 at 1050°C, relative density 55-58%) exhibited *p*-type metallic-like electrical conductivity, 400-500 S/cm at 800-600°C, and a moderate thermal expansion, with average CTE ~13.0 ppm/K at 25-800°C.

Porous $LaNiO_{3-\delta}$ electrodes were applied onto different solid electrolytes, including $(ZrO_2)_{0.92}(Y_2O_3)_{0.08}$ (8YSZ), $Ce_{0.9}Gd_{0.1}O_{2-\delta}$ (CGO10), and $(La_{0.8}Sr_{0.2})_{0.98}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ (LSGM), and sintered at 1050°C for 2h under oxygen flow. The studies of symmetrical cells by EIS demonstrated that the electrochemical activity of $LaNiO_{3-\delta}$ electrodes increases in the sequence 8YSZ < CGO10 < LSGM; the corresponding values of electrode polarization resistance (R_η) at 800°C were 9.5, 4.2 and 0.22 $Ohm\times cm^2$, respectively. Significant variations of R_η with electrolyte composition correlate with the extent of chemical reactivity between $LaNiO_{3-\delta}$ and electrolyte materials during the electrode fabrication. The R_η values of $LaNiO_{3-\delta}$ electrodes in contact with LSGM electrolyte can be further reduced down to 0.03 $Ohm\times cm^2$ at 800°C and 0.11 $Ohm\times cm^2$ at 700°C by the surface modification with PrO_x. The performance of $LaNiO_{3-\delta}$-based electrode layers on LSGM electrolyte under steady-state anodic polarization was evaluated using 3-electrode configuration at 600-800°C.

OR-30

First Principles Evaluation of Photocatalytic Suitability of 2*H* Structured and [0001] Oriented Graphene-like WS_2 Nanosheets and Nanotubes

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Tungsten disulfide (WS_2) 2D nanosheets (NSs) with thicknesses (h_{NS}) from 1 up to 12 monolayers (MLs), and 1D single-walled nanotubes (SW NTs) of different chiralities with diameters d_{NT} > 1.9 nm were found to be suitable for photocatalytic applications since their bandgaps correspond to the range of visible light between the red and violet edges of the spectrum (1.55 eV < $\Delta\varepsilon_{gap}$ < 2.65 eV). For all the studied WS_2 NSs and NTs, the levels of the top of the valence band and the bottom of the conduction band must be properly aligned relatively to H_2O oxidation and reduction potentials separated by 1.23 eV: $\Delta\varepsilon_{VB} < \varepsilon_{O_2/H_2O} < \varepsilon_{H^+/H_2} < \Delta\varepsilon_{VB}$.

The values of $\Delta\varepsilon_{gap}$ decrease with the growth of h_{NS} and increase with the growth of d_{NT} (Fig. 1). 1 ML NS is considered as a limit of infinite growth of SW NTs ($d_{NT} \rightarrow \infty$) and its bandgap increases up to ~2.65 eV. First principles calculations were performed using the hybrid DFT-HF method (HSE06 Hamiltonian) adapted for 2*H* WS_2 bulk [1]. The highest solar energy conversion efficiency (15-18%) expected at $\Delta\varepsilon_{gap}$ = 2.0-2.2 eV (yellow-green range) was found for 2 ML thick (stoichiometric) WS_2 (0001) NS and WS_2 NTs with d_{NT} ~ 3.0 nm (irrespectively on chirality indices *n* of the latter).

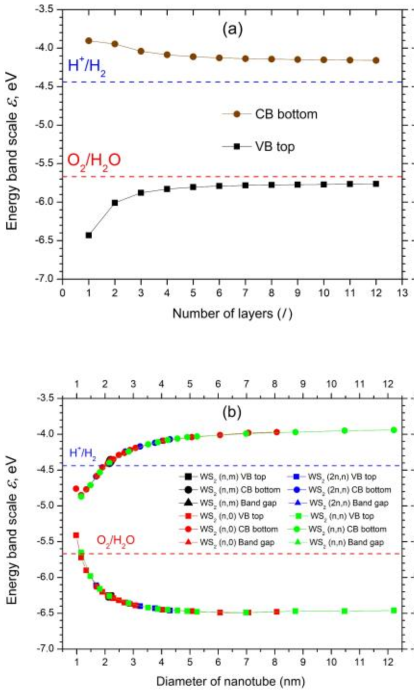

Fig.1. Dependences of $\Delta\varepsilon_{gap}$ edges on varying WS_2 NS thicknesses (a) and diameters of NTs with different chirality (b) aligned along the ε_{H^+/H_2} and ε_{O_2/H_2O}, potentials.

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OR-31

Hydrogen Production by Water- hydrolysis using Graphene Powder Coated with Magnesium

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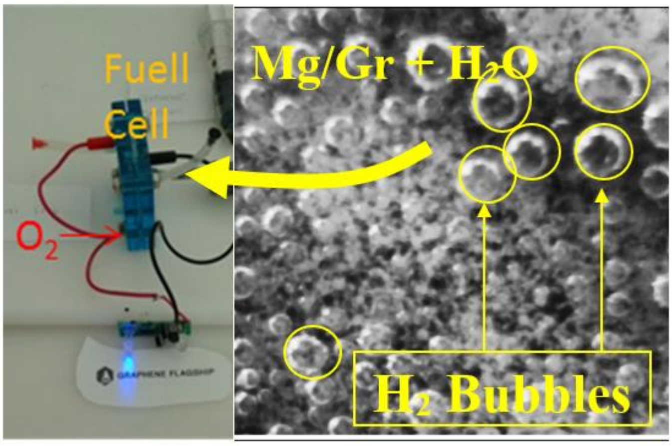
The shortage of non-renewable fossil fuels (petroleum, coal, oil, gas) and the increasing worldwide demand for energy together with the increasing widespread pollution require urgently new methods to produce, convert and store energy. Nanotechnology has opened new perspectives by creating new engineered materials to meet these challenges by improving the efficiency in energy conversion and storage. The latter is considered one of the most important objectives to convert the economy on renewable energy sources. In this respect, water is appealing candidate to store and release hydrogen (H_2) through a metal – water reaction, e.g. magnesium (Mg)-water reaction. This latter is an exciting way to generate hydrogen in situ. Unfortunately, the reactivity of magnesium bulk is not enough good to be used in practical applications. To improve the responsiveness of Mg, various methods can be used such as the reduction of the grain dimension of Mg powder, the addition of corrosive chemical compounds to water, or the increase of the temperature to accelerate the reaction. However, from the practical point of view, a rector working at room temperature and containing only water as reactant is preferable and user-friendly to generate H_2 on-demand. In this work, we studied the use of graphene (G) powder to enhance the reactivity of Mg increasing surface area involved in the reaction with water. Higher values of Mg surface area were obtained by depositing thin magnesium films directly on the Graphene sheets. The depositions on Graphene powder were performed by plasma magneto sputtering. H_2 production have been tested mixing the Mg/Gr powder with water in a cell with pressure sensor. The feasibilility to produce energy by hydrogen produce Mg/Gr in water has been tested a simplified reactor combined with a fuel cell. The findings show that deposition of Mg on graphene using plasma technology is possible and the magnesium deposited on Gr exhibits a high reactivity with water even at room temperature. The hydrogen produce by Mg/Gr nanocomposite material in water has been successfully use in a fuel cell indicating the Mg/Gr powder is a promising material for new concept for on demand energy generation.



OR-32

Relaxation Pathways in Semiconducting Carbon Nanotubes

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We present a thorough analysis of one- and two-color transient absorption measurements performed on single- and double-walled semiconducting carbon nanotubes [1, 2]. By combining the currently existing models describing exciton–exciton annihilation—the coherent and the diffusion-limited ones—we are able to simultaneously reproduce excitation kinetics following both E11 and E22 pump conditions. Our simulations revealed the fundamental photophysical behavior of one-dimensional coherent excitons and non-trivial excitation relaxation pathways. In particular, we found that after non-linear annihilation a doubly-excited exciton relaxes directly to its E11 state bypassing the intermediate E22 manifold, so that after excitation resonant with the E11 transition, the E22 state remains unpopulated. A quantitative explanation for the observed much faster excitation kinetics probed at E22 manifold, comparing to those probed at the E11 band, is also provided.

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OR-33

New Three-body Force-field for Calculation of the Thermodynamic Properties of MoS_2 Nanolayers and Nanotubes

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The thermodynamic properties of the inorganic nanotubes and their temperature dependence can be investigated by ab initio methods [1]. However, this is practically possible only for single-wall nanotubes with diameters less than ≈ 3 nm because of the computer resources shortage. The development of empirical force field models is a computationally efficient solution of the problem. Thus, recently the parameterization of Stillinger-Weber (SW) potential was designed for single-layer MoS_2 [2], which allows the phonon calculations.

In the present study the three-body potential for bulk 2H- and 3R-MoS_2 and related nanosystems is proposed. The potential includes five comparatively simple functional forms. The SW [2] and inverse Gaussian [3] (iG) two-body terms describe the interactions of Mo and S atoms; the iG and Grimme C_6 [4] (G) two-body terms determine the interactions between S atoms in different layers; the SW three-body terms [2] treat interactions of Mo atom with two S atoms and the interactions of S atoms with two Mo atoms. The potential (SW+iG+G≡SWiGG) implies that the MoS_2-based crystalline structures are the systems with predominantly covalent-bonding atoms interactions.

The proposed SWiGG force-field reproduces well the structural, energetic, and phonon properties of the two most common bulk MoS_2 polytypes, monolayer and single-wall nanotubes. The capability of the force field to describe various properties of the lamella-like phases with adequate accuracy encourages its application to modeling of the experimentally observed multi-wall MoS_2 nanotubes.

The preliminary calculation of the MoS_2 nanotubes' thermodynamic properties indicates that the thermal contributions are diminished significantly with nanotube diameter growth from 1.5 to 3.5 nm. It is found that thermodynamic properties of the zig-zag nanotubes are more sensitive to temperature change than those of the armchair nanotubes.

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OR-34

Studies of Magnetotransport and Josephson Supercurrent in Topological Insulator Nanoribbons

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Topological Insulators (TIs) have recently attracted tremendous attention due to their possible application in spintronics and quantum computation. Theory predict that the induced superconductivity in the topological surfaces of TIs host Majorana Bound States (MBS). Signatures of MBS can be experimentally probed in Josephson junctions made with TIs. However, the MBS represent only one of many conventional channels of a Josephson junction. Therefore, a state – of the art Josephson junctions with a few conduction modes are needed. Another limitation is set by the currently available TI materials, where the bulk of material is insufficiently insulating hindering access to the topological surface states.

Nanowires and nanoribbons of TIs are promising to fabricate state of the art Josephson junctions with few cannels. They possess large surface – to volume ratio leading to the suppression of the material bulk and a decreased number of conduction modes.

Here we present a characterization of charge transport in Bi_2Se_3 nanoribbons by magnetotransport measurements, such as Hall effect in a single nanoribbon, Aharonov-Bohm and Shubnikov-de Haas oscillations and their gate gate dependencies over a wide range of nanoribbon thicknesses. Three main charge carrier contributions to the transport have been identified; namely – topological surface carriers, bulk carriers and carriers from accumulation layer at the nanoribbon interface with substrate. Nanoribbons with thicknesses below 30 nm enter *bulk-free* regime. Here carriers from the bulk are fully suppressed and only surfaces and 2DEG from accumulation layer defines the total charge transport.

Josephson junctions have been defined by patterning a nano-gaps of Al on *bulk – free* Bi_2Se_3 nanoribbons. We detect clear sub – gap features arising from multiple Andreev reflections, highlighting high transparency of TI/superconductor interfaces. Josephson current in response of magnetic field shows a Fraunhofer – like modulation and irradiation with an *rf* excitations gives a Shapiro steps with a hint of a 4π periodic supercurrent contribution.

OR-35

Synthesis and Magnetotransport Properties of the Multilayered Quasi-one-dimensional Nanostructures

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Recently a large interest in the field of study of magnetic nanostructures: multilayer films [1], quasi-one-dimension structures or nanowires [2] was observed due to both as scientific significance and as prospects for practical application. Nanosized multilayered metal structures are characterized by the negative magnetoresistive effect - drastic reduction of the electrical resistance under magnetic field [3]. It is connected with the alignment of the magnetizations in magnetic layers (transition from antiparallel to a parallel ordering) under magnetic field. Multilayered quasi-one-dimensional structures (MQODS) are excellent model for explanation magnetotransport phenomena in magnetic nanomaterials. MQODS were obtained in the pores of the anodic aluminum oxide (AAO) templates with pore diameter 100-200 nm via electrolyte deposition [3]. Each nanowire consists of huge number of alternating nanosized ferromagnetic (CoNi alloy with thickness 25-350 nm) and diamagnetic (Cu with thickness – 2-5 nm) layers. The length of MQTDS varied from 13.5 μm to 60 μm.

Our investigations demonstrate that value of the MR in MQODS depends on many factors: ratio of 'length/thickness' of the nanowires, the number and thickness of the ferromagnetic and diamagnetic layers, temperature. Magnetoresistive coefficient (GMR) of MQODS as a function of 'length/thickness' ratio and diamagnetic layers thickness was investigated. It has been shown that GMR value increases (from -1.9 % to -13 %) with increasing of the nanowires length (from 13.5 μm to 60 μm). This is due to the cumulative effect of increasing the number of alternating layers and an increase in the ratio 'length/thickness' of nanowires. It has been also shown that the thickness of diamagnetic layers (as an interface layer and a chemical purity) is the most decisive factor. With Cu layer thickness decreasing from 5 nm to 2 nm negative GMR increased from -13 % to -27.6 % respectively. It causes by stronger interaction of spin-polarized electrons in the magnetic layers via RKKY exchange.

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OR-36

Carbon Nanotubes vs Graphene Nanoplatelets for 3D-printable Composites

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Polymer-based composites with nanocarbon fillers are of great interest for the wide application range. However, the composite properties such as excellent electromagnetic energy dissipation or tailorable conductivity are not enough to solve practical problems in engineering. To be fully applicable, the composite material must be economic and suitable for standard methods of fabrication such as 3D-printing.

Investigated composites were based on PLA (polylactic acid) polymer which is commonly used as a 3D-printing filament. Multi-wall carbon nanotubes (MWCNT) and graphene nanoplatelets (GNP) were used as composite fillers.

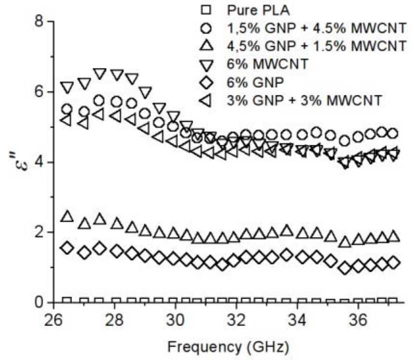

Fig.1 Imaginary part of permittivity for PLA-based composites with different concentrations of MWCNT and GNP fillers

Homogeneous samples of nanocomposites were investigated in 0.01 – 18 and 26 – 37 GHz ranges. Samples with equal weight concentrations of MWCNT and GNP have close values of *ε'* but the first one (filled with 6 wt % of MWCNT) has significantly higher value of *ε"* (Fig. 1). Such a difference in complex permittivity behavior allows customizing the electromagnetic response by changing the filler concentration.

Acknowledgements: this work is supported by H2020 RISE 734164 Graphene 3D project.

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ABSTRACTS
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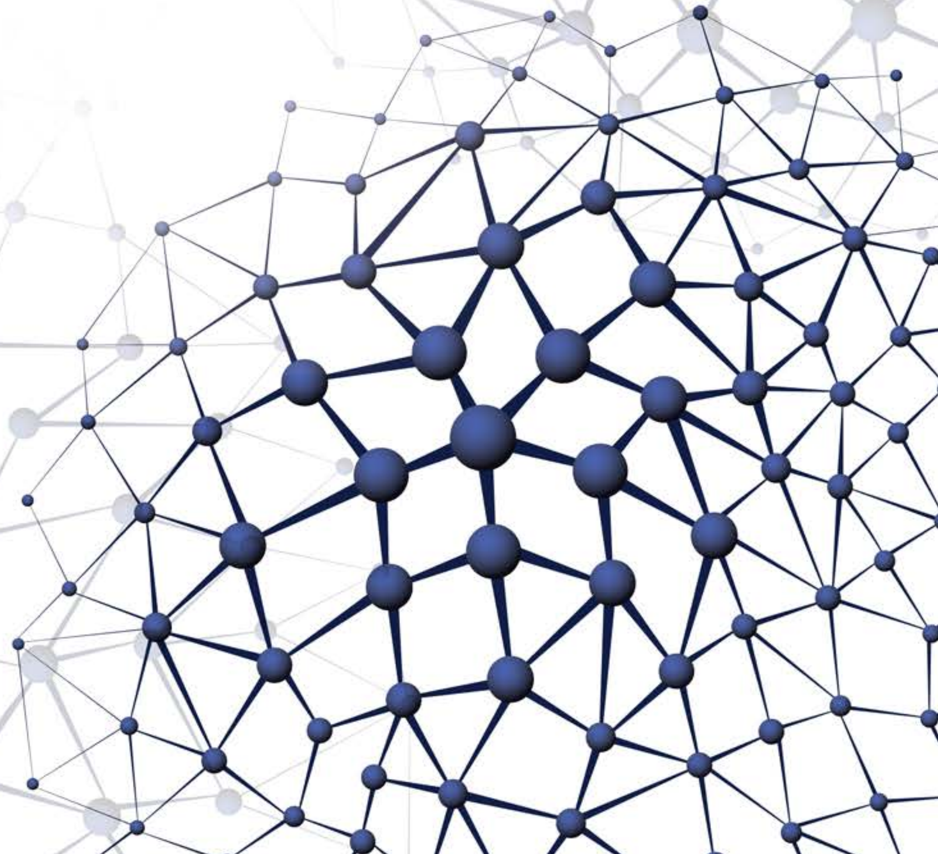

PO-1

Comparative First-principles Calculations of ZrS_2 and HfS_2-based Nanotubes

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The synthesis of nanomaterials with unusual properties based on carbon nanotubes and fullerenes stimulated numerous theoretical and experimental studies to find their possible analogs on the basis of other compounds. Particularly, it was demonstrated that nanotubes produced from layered transition metal disulfides exhibit a stable, closed, hollow structure. Among the other transition metal disulfides, ZrS_2 and HfS_2 have attracted a significant attention because of their unique electronic features resulted in numerous applications in photocatalysis and electrochemical intercalation. [1, 2].

We performed a theoretical study on the structure, stability, and phonon frequencies of monolayers and nanotubes based on Zr and Hf disulfides. First-principles calculations were made using the hybrid exchange-correlation functional HSE06 and LCAO approximation implemented in the computer program CRYSTAL-2017 [3].

The simple for practical applications approach to symmetry analysis of infrared- and Raman active vibrational modes in ZrS_2 and HfS_2 nanotubes is suggested. It is shown that the number of IR and Raman active modes is constant for NTs with the same chirality type. The correlation of the phonon modes of nanotubes with those of monolayer is analyzed.

Thermodynamic functions for monolayers and nanotubes with various chirality and diameters are calculated for the first time on the basis of the obtained phonon frequencies. It is found that the phonon contribution to the nanotube folding energy is small, but it is important for an accurate estimate of the stability of nanotubes of small diameters. Calculated results show that thermal contributions to Helmholtz free energy are positive; thereby they reduce the stability of ZrS_2 and HfS_2 nanotubes especially at elevated temperatures.

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PO-2

Comparative Study of Phonons and Thermodynamic Properties of MoS_2 and WS_2 Nanotubes

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The disulfides of transition metals MS_2 (M = Mo, W) are a subject of extensive experimental and theoretical studies of the stability, electron due to many useful applications, such as rechargeable lithium-ion batteries and electrochemical hydrogen storage devices.

It is so far performed many quantum-chemical calculations of the electronic structure and stability of nanolayers and nanotubes based on disulfides of transition metals. Nevertheless, there are practically no calculations of their thermodynamic properties, such as an entropy S, Helmholtz free energy F and a heat capacity C_V.

In our previous work [1], hybrid DFT calculations were made for the first time on the phonon dispersion and thermodynamic properties of WS_2-based single-wall nanotubes. We have obtained the temperature dependence of the free energy, entropy, and heat capacity of WS_2 nanotubes. In the present work, we report the results of our first-principles comparative study of the phonon and thermodynamic properties of MoS_2 and WS_2 nanotubes. The phonon dispersion of bulk, monolayer, and achiral single-wall nanotubes are calculated within a full symmetry approach implemented in the CRYSTAL14 computer code.[2] Using the *ab initio* method, we compare the temperature dependence of the thermodynamic functions of nanotubes MoS_2 and WS_2 at the first time.

In summary, phonon frequencies obtained both for the layers and nanotubes are used to compute the thermal contributions to thermodynamic functions. It is found the noticeable deviations in the thermodynamic properties of thin MoS_2 and WS_2 nanotubes in regard to monolayer properties. It is also shown that the thermal contribution to the strain energy of nanotubes is appreciable, especially for nanotubes with small diameters, and increases their relative stability with temperature. The deviation of nanotube free energy, entropy from the corresponding layer values is larger in the case of MoS_2 than in the case of WS_2.

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PO-3

Atomistic Scale Modelling of Modern Materials Using ACELAN Package

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In this paper we use ACELAN package [1] which is modern finite element software designed for solving complex problems of computational physics and for material properties identification. As a part of modification procedures it was decided to develop ACELAN-COMPOS package with the possibility to work with nanoscale identification models.

At the moment those nanoscale models are carbon based models [2] and zinc oxide (ZnO) samples [3,4]. All models have the same principle of the samples' building. As input data one can use desired size, interaction potential and for carbon based models also the shape (graphene sheets or tubes). After input data ACELAN-COMPOS performs an identification process.

For ZnO samples we identified a set of its elastic and piezo constants. Point of interest of that problem was to prove the size effect – the dependence of the piezo constant on the sample's size. As shown in Fig. 1, this task was done well. ZnO was chosen because of its unique properties and the relative simplicity of crystals growing. For carbon structures it is possible to identify the set of elastic constants and to build amplitude-frequency characteristic.

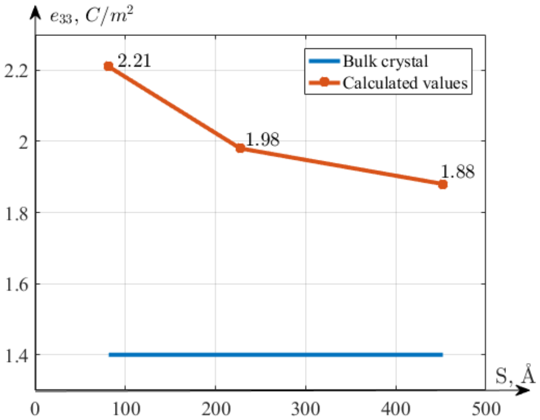

Fig.1 Calculated dependence of the e_{33} constant on the size of the basement, S, of ZnO nanorod. With increasing of the basement size the constant e_{33} tends to its bulk value.

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PO-4

The Influence of Impurities on the Formation Energies of Point Defects in Ti-Al Alloys

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Intermetallic Ti-Al alloys and alloys based on these compounds are materials of high technological importance. These alloys have unique mechanical properties such as a high specific strength, advanced creep characteristics and relatively good oxidation/corrosion resistance. The development of high-temperature structural materials on the base of Ti-Al alloys whose properties are between nickel-based superalloys and high-temperature ceramics is the important task of modern materials science. It is well known that the mechanical properties of the engineering alloys are related directly to the atomic diffusion. All self-diffusion mechanisms need existing some point defects or their complexes. In present work as the first step towards deeper insight of the self-diffusion mechanisms, the formation energies of point defects in the Ti_3Al, TiAl and $TiAl_3$ alloys are investigated by the projector augmented-wave method within density functional theory. It is shown that antistructural defects are the dominant ones irrespectively of alloy composition. The effective formation energies of point defects in γ-TiAl are shown in Fig. 1. In the set of Ti_3Al-TiAl-$TiAl_3$ the formation energy of Al-vacancy decreases by ~1.3 eV with increase of Al content whereas the formation energy of Ti vacancy changes insignificantly. It was found that the formation of Ti-vacancy needs lower energy than Al-one in all considered alloys. Site occupancies of 4d and simple metal impurity atoms in Ti-Al alloys are calculated. The influence of impurities on defect formation energies and elastic constants is discussed. The activation energies for atomic diffusion in TiAl are found to be in agreement with experiment.

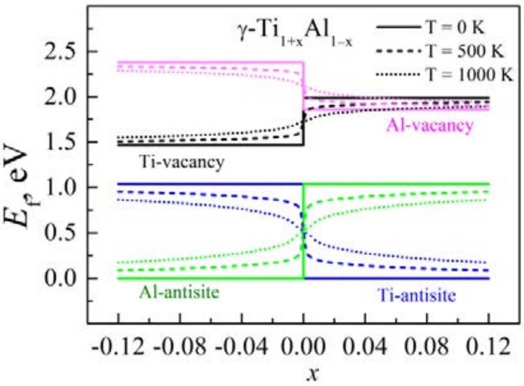

Fig. 1. Effective defect formation energy as function of deviation from stoichiometry composition for different temperatures.

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PO-5

Influence of Fluorine and Oxygen Adsorption on Electronic Structure of InSb(111) Surface

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The progress in manufacturing of devices based on $A^{III}B^{V}$ semiconductors is connected with the development of a special technique which provides the low density of states at insulator–semiconductor interfaces. Controlled growth of fluorine-containing anodic oxide layers (FAOL) in different liquid and gas media is one of the ways to modify a semiconductor surface to create metal–insulator–semiconductor structures. The complex composition of the FAOL/$A^{III}B^{V}$ interface transition region considerably complicates finding out the microscopic nature of interface states. In this connection *ab-initio* calculations, which allow to understand the origin of interface states and chemical bonds of adsorbate at semiconductor surface, are actively used.

In present work we discuss the influence of O and F adsorption as well their coadsorption on the electronic properties of the InSb(111) surface. The calculations were performed by the projector augmented-wave method within DFT along with the hybrid functional HSE method. Investigation of the electronic structure was carried out by. Our results demonstrate that there is a surface state in the band gap, which is pinning the Fermi level in case of the InSb(111) unreconstructed surface (Fig. 1a). Oxygen adsorption on the surface leads to the appearance of additional states in the band gap (Fig. 1b) the structure of which depends strongly on an adsorbate site on the surface. In case of fluorine adsorption the charge of the Sb subsurface atom changes insignificantly that can explain the absence of its unoccupied surface states in the band gap. It is shown that the O-induced surface states can be completely or partly removed from the band gap by fluorine coadsorption.

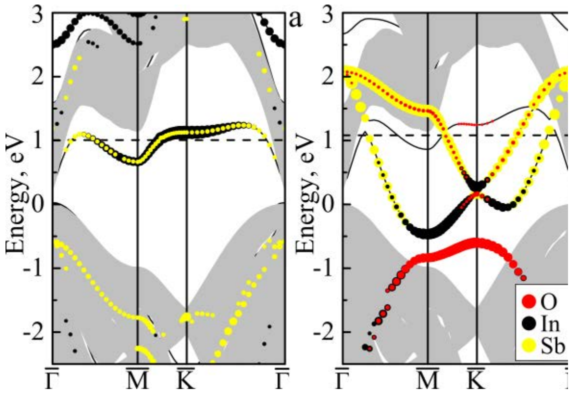

Fig. 1. Electron energy spectra of the unreconstructed InSb(111)-(1×1) surfaces (a) and the surface with oxygen absorbed in the Sb_2 site (b).

The work is partly supported by the TSU Competitiveness Improvement Program.

PO-6

CO_2 Adsorption on Mixed Ionic-Electronic Conducting Membranes

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Major sources for human-made CO_2 emission comprise the energy and the industrial sector including cement production. One of the most appropriate concepts to capture CO_2 from fossil plant exhausts is the oxyfuel combustion. However, most of known highly permeable ceramic membrane materials show unwanted chemical instability against CO_2 and other flue gas components. Therefore, new advanced mixed ionic-electronic conducting membrane materials and components are needed for such technological processes as the oxyfuel combustion.

We performed detailed theoretical study of the effect of CO_2 gas on surface properties of the (La,Sr)FeO_3 perovskite membranes based on the state-of-the-art hybrid density functional (DFT) calculations with and without the inclusion of dispersion interactions (DFT-D3 [1]) as implemented into latest CRYSTAL17 computer code [2]. Such hybrid DFT calculations allow us for a deeper atomistic understanding of the CO_2 adsorption. This includes the correlation between the adsorption enthalpy and stability of different atomic configurations for the CO_2 molecule adsorption and membrane basic properties, such as the Fe oxidation state, a role of surface vacancies, carbonate formation, charge redistribution near surface and chemical bond lengths and bond populations.

The calculated hybrid DFT CO_2 adsorption enthalpies are compared with those estimated from experimental oxygen permeation tests. Their good agreement indicates at important role of surface oxygen vacancies and confirmed the formation of carbonate phases.

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PO-7

Negative Thermal Expansion of ScF_3: First Principles vs Empirical Molecular Dynamics

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ScF_3 is an interesting material exhibiting negative thermal expansion (NTE) property over a wide range of temperatures from 10 to 1100 K. In this work, the NTE of ScF_3 is studied using two different approaches based on empirical and first principles molecular dynamics as realized in the CP2K code [1]. The temperature dependence of the average lattice constant within an NPT ensemble, inter-atomic angle distributions for Sc-F-Sc atomic chains, and radial distribution functions were calculated.

We have compared the results of empirical versus first principles molecular dynamics calculations and cross-checked them with gathered theoretical and experimental data for ScF_3 available in the literature [2, 3, 4]. Our results suggest that the first principles MD calculations are able to reproduce qualitatively the negative thermal expansion effect in ScF_3, which is attributed to the tilting motion of ScF_6 octahedra. The results of the MD simulations were also validated by a comparison with the Sc K-edge X-ray absorption spectra [5].

The advantages and limitations of both MD approaches are discussed.

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PO-8

Simulation of the Band Structure and Density of States of the Nanocrystal NaCl

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Currently, the properties of alkali halide nanocrystals have attracted great interest from experts in chemistry, physics, and engineering. They are simultaneously regarded as fundamental objects in which the molecular and solid properties are reflected [1,2].

With the help of computer simulation, the band structures of NaCl nanocrystal at 1 K were calculated. The calculated minimum width of the band of forbidden energies for a chain of two ions is 10.25 eV, of four –11.4 eV, of six– 8.449 eV and of twelve – 10.46 eV.

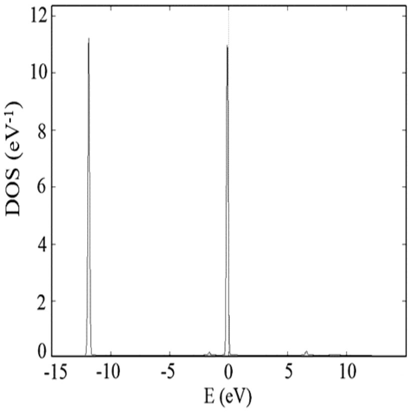

Fig.1 Density of *s* state of NaCl, consisting of one sodium ion and one chloride ion

The lowest valence band occurs mainly from the *s*-orbit of Cl halogen, while the chlorine *p*-orbit is very weakly bound to the *p*-state of Na, as can be seen from the density-of-states plot. In figure 1 we observe two peaks responsible for *s*-orbits. The peak near -12 eV is connected with the halogen Cl, and the peak in the vicinity of 0 eV is connected with Na.

The calculated minimum width of the band of forbidden energies for NaCl constructed on a plane of four ions is 11.83 eV, of six – 11.46 eV, of eight – 11.55 eV and of twelve – 12.09 eV. The calculated minimum width of the forbidden energy band for bulk NaCl constructed from eight ions is 11.92 eV and from twelve to 11.12 eV.

Thus, the results of computer simulation of the band structure, the density of states, and the total energy of a NaCl nanocrystal in various cluster compounds (NaCl, Na_2Cl_2, Na_3Cl_3, Na_4Cl_4, Na_6Cl_6), depending on the geometric arrangement of ions in space at 1 K. Modeling features implemented in the program Atomistix ToolKit with Virtual NanoLab. It is revealed from the characteristic form of the density of states that these objects should be referred to quantum dots.

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PO-9

First Principles Calculations for Polar $YAlO_3$ (001) Surfaces

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The results of *ab initio* calculations of polar $YAlO_3$ (001) surfaces by means of a hybrid B3LYP exchange-correlation functional as it is implemented in the CRYSTAL computer code are presented. Both polar YO and AlO_2-terminations of the cubic $YAlO_3$ (001) surface were considered. We performed relaxation of atoms on the upper three layers of both YO and AlO_2-terminated $YAlO_3$ (001) surfaces using slabs containing 22 and 23 atoms and 9 layers, respectively. The Al-O chemical bond covalency change near the AlO_2-terminated $YAlO_3$ (001) surface relative to the $YAlO_3$ bulk is discussed. YO and AlO_2-terminated $YAlO_3$ (001) polar surface energies are calculated and compared with ABO_3 perovskite (001) surface energies [1-9]. Our B3LYP calculated electronic band gaps of the YO and AlO_2-terminated $YAlO_3$ (001) surfaces are compared with the $YAlO_3$ bulk band gap.

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PO-10

Quantum Paraelectric State in $(Pb_ySn_{1-y})_2P_2S_6$ Crystals

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Mixed crystals with sulfur by selenium substitution or with tin by lead replacement can be grown in all the concentration range. It is clear that substitution greatly changes physical properties of the crystals and gives possibility to observe new phenomena.There are two main reasons of the interest to study this crystal within the $(Pb_ySn_{1-y})_2P_2(Se_xS_{1-x})_6$ system. First is the vicinity of the Lifshitz point on $T-x$ diagram in substitution of sulphur for the selenium, when the phase diagram splits into two lines. The second point of interest is that on $p-T$ diagram the transition temperature decreases with concentration of lead up to 0 K and reaches value y = 0.61 for sulphur series and value y = 0.4 and y = 0.64 for selenium series, respectively.

For $(Pb_ySn_{1-y})_2P_2S_6$ mixed crystals with compositions that are close to the transition at zero temperature from polar phase, the dielectric susceptibility demonstrates the quantum critical behavior $1/\varepsilon \sim T^2$ in vicinity of the phase transitions. It is interesting to understand the nature of quantum paraelectric state in $(Pb_ySn_{1-y})_2P_2(Se_xS_{1-x})_6$ mixed crystals. In this contribution, we present dielectric results of $(Pb_ySn_{1-y})_2P_2(Se_xS_{1-x})_6$ mixed crystals with germanium impurities. The dielectric constant of the investigated samples were measured between 20K and 300K. Their temperature dependences were analyzed on the basis of the Barrett model.

PO-11

Modeling of F-type Centers Thermal Annealing in Neutron Irradiated and Thermochemically Reduced BeO

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The radiation-resistant binary oxide BeO, is one of the very important materials for applications in fusion reactors.

In this work, we analyzed the kinetics of the F-type and V center annealing after neutron irradiation. F-type center kinetics were treated as the bimolecular process with equal concentrations of the complementary F and Oi defects. Such process is controlled by the interstitial oxygen ion mobility, which is much higher than that of the F centers. The F center annealing begins at temperatures 500-700 K, when both F and F+ centers are practically immobile, due to the recombination with mobile Oi defects. It is demonstrated how the shape of the F-annealing curves is determined by two control parameters: Ea and effective pre-exponential factor and strongly depends on irradiation conditions.

Special attention is paid to a detailed comparison of diffusion-controlled F center thermal annealing in neutron-irradiated BeO with similar data obtained for for MgO, Al_2O_3 and $MgAl_2O_4$ [1-3]. The results obtained are used for the evaluation of interstitial oxygen migration parameters and are compared with the available *ab initio* calculations for MgO and Al_2O_3.

Finally, we also treated the kinetics of F-center annealing in thermochemically-reduced BeO crystals. The obtained activation energy allows toevaluate both the intrinsic F-center migration energy and also the conditions for metal colloid formation in BeO.

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PO-12

Lattice Dynamics of White Phosphorus

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Phosphorus exist as white, black and red allotropes at ambient conditions. White phosphorus at ambient conditions (α form) consists of P_4 tetrahedra arranged in the body centered cubic crystalline lattice.

In our work, the dynamics of the crystalline lattice of white phosphorus is studied. The calculations of the crystal lattice vibrations were made using the molecular dynamics calculation program GULP. The parameters for the interaction of phosphorus atoms were obtained using the experimental IR and Raman spectra and the theoretically calculated lattice vibration frequencies. Theoretical vibration frequencies were obtained in DFT calculations using the CRYSTAL14 program. There are several characteristic areas in the spectrum of variations: the internal vibrations of the P_4 molecule at 360 cm^{-1}, 460 cm^{-1} and 600 cm^{-1} and the lattice and libration vibrations below 120 cm^{-1}.

PO-13

Structural and Electronic Properties of Pure and Ce3+ Doped β-NaYF4

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Hexagonal NaYF4 doped with Ce^{3+} and other rare-earth ions is one of the most popular up-conversion phosphor materials [1,2]. Due to low phonon energy and multisite structure it has high luminescence efficiency [3]. Such ABF_4-type fluorites are also considered as a potential material for high-energy physics [4].

In this work we present simulations on hexagonal β-NaYF4 using density functional theory (DFT) approach with linear combination of atomic orbitals (LCAO) implemented in CRYSTAL14 code. According to literature data, three possible space groups of this compound were discussed: P-6, $P6_3/m$ and P-62m. Firstly, we have modelled disordered crystal structure of NaYF4 within the large supercell containing 108 atoms. To get a better agreement with experimental data different exchange-correlation functionals have been tested: HSE06, PWGGA and PWGGA+13%HF. It was found that for all three functionals, the minimum of total energy corresponds to P-6 space group. Vibrational frequencies and Raman spectra was calculated for lowest energy structure and compared with available experimental data.

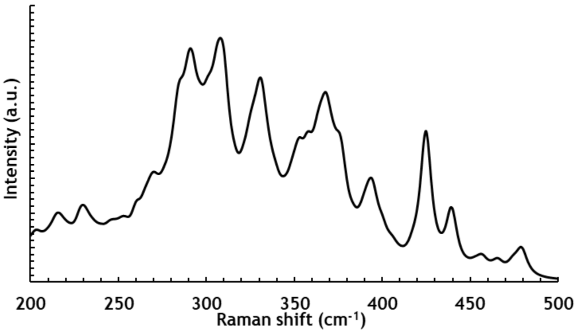

Figure 1 Calculated Raman spectra of $NaYF_4$ P-6 phase powder at 293 K temperature

In the second part of our study, we have simulated P-6 β-NaYF4, with introduced fluorine vacancies and $Ce_{Y/Na}^{3+}$ substitute ion, or both together. For successful treatment of Ce^{3+} in β-NaYF4, we performed a series of calculations, where Ce^{3+} ion was substituting Y atom in different positions. The obtained structures were used for further calculations, where nearest to Ce^{3+} fluorine atom was removed, to simulate F-center. For all defects, formation and incorporation energies were calculated.

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PO-14

Stability and Mechanical Properties of Al_2O_3/Ti_3Al Interface

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Intermetallic Ti-Al alloys and alloys based on these compounds have high technological importance due to unique mechanical properties. To expand treir technological applications, the development of new structural materials the mechanical properties of which would be between the properties of high-temperature ceramics and nickel-based superalloys is needed. In this connection it is necessary to understand better the mechanism of surface oxidation of Ti-Al alloys at the microscopic level. Experimental studies have shown that low corrosion resistance of the Al-poor alloys is connected with a growth of mixed oxide layers containing titanium and aluminum oxides. It has been established that in spite of the initial oxidation stages of titanium aluminides may differ depending on the aluminum content, at the later stages internal and external oxidation takes place simultaneously. The outer oxide film is mainly formed by titanium dioxide (TiO_2), whereas alumina (Al_2O_3) is formed at the alloy- oxide interface. The purpose of the work is to study the properties of internal Al_2O_3/Ti_3Al interface which is formed due to Al depletion of interface Ti-Al layers.

The energy preferred interface $Al_2O_3(0001)_O/Ti_3Al(0001)$, which is characterized by the highest adhesion of ~11 J/m^2, is formed on the O-termination of the alumina surface. A significant increase in the adhesion energy is due to the large ionic contribution to the chemical bonding at the interface. In this case the interface energy is smale and even becomes negative with an increase in the oxygen concentration. This indicates the preference of oxygen segregation to the Al_2O_3/Ti_3Al interface and, consequently, further oxidation of the alloy. Hence, the slowing of the diffusion of oxygen through the oxide layers is an effective method to improve the corrosion resistance of titanium aluminides. This effect can be achieved by doping. It has be shown by *ab initio* methods some impurities such as Zr, Nb, Mo, Hf, Ta, W, Re segregating into the oxide increase the formation energy of oxygen vacancies.

The work is supported by the Russian Foundation for Basic Research under grant N 18-03-00064_a and the TSU Competitiveness Improvement Program.

PO-15

Ab initio Simulation of (Ba,Sr/Ca)TiO_3 Composite Perovskites

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An enhancement of the electromechanical properties of lead-free materials, which allow mutual conversion of mechanical and electrical energies and may be used for different commercial applications, including energy harvesting, is the challenging problem. Progress in material engineering allows producing new complex materials with improved ferroelectric and piezoelectric properties. For example, to optimize the electrical properties of the widely applicable $BaTiO_3$ (BTO) perovskite, the chemical substitution of Ba ions by isovalent dopants may be used.

In this work, we considered (Ba,Sr)TiO_3 [1] and (Ba,Ca)TiO_3 solid solutions. The results of the first-principles computations of electromechanical properties are presented and discussed. Supercell calculations were performed with CRYSTAL14 code [2] within the linear combination of atomic orbitals (LCAO) approximation, using two advanced hybrid functionals (PBE0 and B1WC) of the density-functional-theory (DFT). Different chemical compositions (dopant/Ba ratio) and spatial arrangements (positions of dopant atoms in supercell) are considered for the ferroelectric phase. Calculated structural properties of solid solutions in tetragonal phase are compared with experimental data and earlier theoretical results. The local structure relaxations for different dopants are compared and discussed. Elastic and piezoelectric constants for concentrations 0%, 12.5% and 25% of dopant atoms relatively of Ba atoms (within ferroelectric tetragonal phase) were calculated in considered solid solutions. It is predicted that piezoelectric properties of solid solutions are improved with increase of dopant concentration, what is important for technological applications.

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PO-16

Magnetic Properties of Solid Solutions $LaGa_{(1-x)}Fe_xO_3$ and $LaAl_{(1-x)}Fe_xO_3$: First-Principles Study

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In recent years, perovskite-type oxides have attracted great attention due to their wide range of applications as advanced materials for solid oxide fuel cells, sensors, electrochemical devices, etc. Fe - doping in the lanthanum gallate against lanthanum aluminate leads to the formation of Fe-clusters. The reasons of such differences are still not determined [1].

Quantum chemical simulations were carried out in order to investigate the magnetic properties of solid solutions. Calculations were performed with CRYSTAL14 within CO LCAO approximation. Our research shows that properties of the bulk crystals calculated with hybrid 9% HF-DFT functional PBE [2] are in good agreement with experimental data. We used supercells composed of 8 to 27 primitive cells to model the solid solutions. The high-temperature cubic and low-temperature orthorhombic ($LaGaO_3$) and rhombohedral ($LaAlO_3$) phases have been explored. All configurations with different spin distribution were split into symmetry independent classes (SIC). Optimized geometry, energy and electron properties were calculated for the representative structure of each class. Estimation of statistical weights allows us to find out the most probable structures of solid solution with the specific local magnetic ordering.

In the first stage of our study the computational scheme was verified by the calculations of properties of $LaGaO_3$, $LaAlO_3$ and $LaFeO_3$ pure crystals in three different polymorphic modifications (*Pbnm, R*-3*c, Pm*-3*m*). Further calculations were performed for 50% and 25% solid solutions $LaGa_{(1-x)}Fe_xO_3$ and $LaAl_{(1-x)}Fe_xO_3$. It was established that in all cases the relative total energy of any spin configuration within the given SIC is directly proportional to the number of atomic triples Fe(↑)–O–Fe(↓) with the opposite spin projection on the Fe atoms. Nevertheless, the energy distribution over the spin configurations is sharp for $LaGaO_3$ solid solutions and wide for $LaAlO_3$ solid solutions. Thereby, the spin polarization affects the local structure of doped lanthanum gallate and lanthanum aluminate differently.

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PO-17

Revealing Conduction Pathways in Solid Lithium Electrolytes by Total Scattering X-ray and Neutron Diffraction Measurements Using Molecular Dynamics Simulation and RMCPOW Methods

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Having a knowledge on the conduction pathways in the electrolyte material of lithium-ion batteries and blocking/facilitating mechanism of conduction at atomic level might help to design better devices.

Total scattering X-ray and neutron diffraction is a valuable tool in this sense. The Bragg-scattering part provides information on the average structure, so conduction pathways is mapped easy. Moreover, diffuse scattering part contains information on the short range order correlations, which is useful to do investigation on the mechanism.

In the present study the crystalline phases of $LiAlCl_4$, $LiClO_4$ and $LiPF_6$ are investigated, which constitute the electrolyte material (the superionic conductor is dissolved in a polymer matrix) of most commercial lithium-ion batteries. The combination of molecular dynamics and Reverse Monte Carlo for POWder[1] simulation procedure used to provide that kind of 3 dimensional structural models, which are consistent with the measured powder X-ray (BL04B2, SPring-8, Japan) and neutron (MTEST, Budapest Neutron Centre, Hungary) diffraction datasets and reasonable concerning energetics. The resulting particle configuration has been analyzed to reveal the conduction channels, the cation-anion and anion-anion correlations (partial pair distribution functions, angular distributions, orientation correlations) at atomic and molecular levels, as well.

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PO-18

Dipole-induced Disorder in Quasi-equilibrium Assemblies of Ferroelectric Nanocubes

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Efficient ambient energy scavenging exploiting piezo-/pyroelectric properties of ABO_3 perovskites to power low-energy devices is an attractive green energy solution. In turn, the colloidal processing of nearly monodisperse and highly crystalline single-domain nanocubes of $BaTiO_3$ is a promising route to produce superlattice assemblies for integration into nanostructured ferroelectric devices [1]. Controlling the local behaviour of ferroelectric nanocrystals is imperative for fabricating highly-ordered assemblies, for energy harvesting solutions among others. The current picture of the nanoscale polarization in individual nanocrystals [2] suggests a potential presence of significant dipolar interaction. However, the understanding of the role of the dipole-dipole interaction in the condensation of ferroelectric nanocubes remains far less advanced.

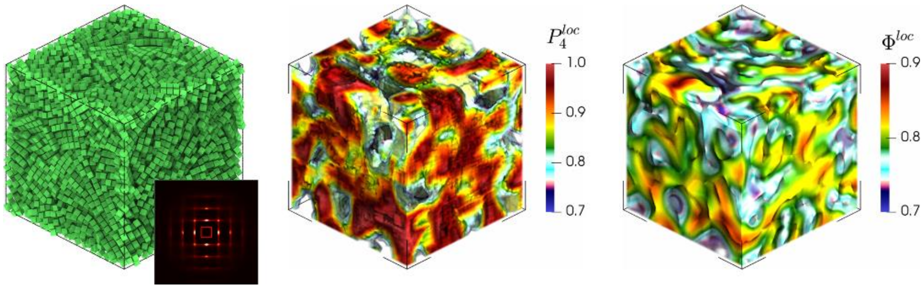

Fig.1 Pressure-induced assembly of approx. 16 000 dipolar nanocubes: Left – simulation snapshot; distributions of cubatic order (middle) and porosity (right).

We will report the microstructural characterization of densified quasi-equilibrium assemblies of ferroelectric nanocubes obtained *via* numerical simulations exploiting discrete element method (DEM) coupled with particle-particle particle-mesh (P^3M) approach for computing long-range dipolar interactions. Our results suggest that the long-range positional and orientational correlations seem to be highly sensitive to the presence of anisotropic (e.g. dipolar) interactions.

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PO-19

Computer Simulation of Cu_n@graphene (0001) Nanostructures for the Electrocatalytic Production of C_2H_4O

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Substitution of fossil-based chemical processes by the combination of electrochemical processes driven by sources of renewable energy and parallel use of H_2O and CO_2 as a carbon source must direct chemical production of bulk chemicals and fuels. The ultimate aim of our study is development and design of a prototype electrochemical reactor combining cathodic CO_2-reduction to ethylene and anodic H_2O oxidation to hydrogen peroxide. In the current presentation, we report on the simplest atomistic 2D graphene-based models (Fig. 1) with attached copper nanoclusters of different configurations, both neutral and charged, in presence of CO_2 and H_2O complexes considered for first principles simulations of various elemental electrocatalytical reaction steps. Fig. 1 shows the schematic representation of fully optimized Cu_n/graphene (0001) two-dimensional (2D) nanostructures with 5-faceted Cu_6 (Figs.1 a,b) and 6-faceted Cu_7 nanodot (Figs.1 c,d). The latter allows us to exploit maximum of symmetry operators and, thus, to drastically reduce the computation time. The applicability of the model nanostructures for computer simulation of electrical conductivity of charged Cu_n/graphene (0001) surface is reported as well.

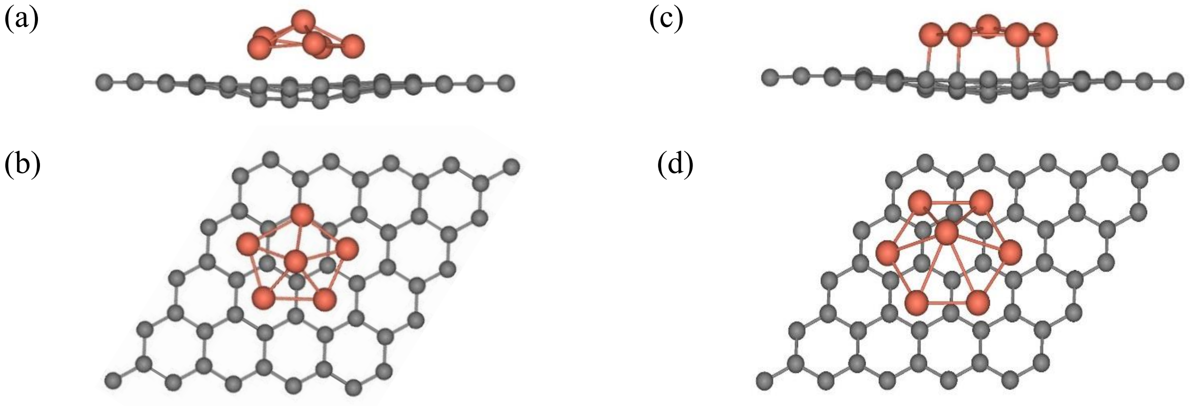

Fig.1. Aside (a) and top (b) views of 5-faceted pyramidal Cu_6 nanodot deposited atop graphene (0001) monolayer as well as aside (c) and top (d) views of 6-faceted pyramidal Cu_7 nanodot atop graphene.

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PO-20

Improved Electrochemical Performances Derived From Synergistic Effect of Reduced Graphene Oxide and TiO_2/Fe_2O_3 in Various Proportions Served as Lithium-Ion Battery Anode

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Lithium-ion batteries (LIBs) and improvement of their effectivity have obtained much attention in the manufacturing of portable electronic devices. Therefore, it is essential that the future LIBs can display the properties of high energy density, excellent charge - discharge stability, high safety, environmental friendly and low cost.

We report an rGO/Fe_2O_3/ TiO_2 ternary nanocomposite with a various proportions of Fe_2O_3 and TiO_2 obtained via spray pyrolysis method followed by reduction of GO (Ar/H_2 flow, 750°C). The proportions of Fe_2O_3 and TiO_2 in anode material are listed in Table 1.

Table 1. Proportions of components in anode material.

Samples	Fe_2O_3 , %	TiO_2 , %	rGO , %
FTGO801010	80	10	10
FTGO702010	70	20	10
FTGO603010	60	30	10
FTGO504010	50	40	10

Scanning electron microscopy (SEM) image in Fig. 1 clearly depicts that, Fe_2O_3 nanoparticles with and TiO_2 nanoparticles with a size of ~50 and 21 nm (nanopowder Aldrich Chemistry), respectively were uniformly surrounded by rGO (BGT Materials, concentration 1 mg/ml, flake size 1–20 µm). Electrochemical properties of all samples were studied by chronopotentiometry, cyclic voltammetry and electrochemical impedance spectroscopy. Structure and morphology investigations were performed by SEM, AFM, XRD and Raman spectroscopy. The results of this study indicate that the rGO/Fe_2O_3/TiO_2 ternary nanocomposite with a material stoichiometric ratios 60 % of Fe_2O_3, 30 % of TiO_2 and 10 % of rGO holds great promise as a high performance anode material for Li-ion batteries, however, the evidence and the reason for this is under investigation and will be reported in the near future.

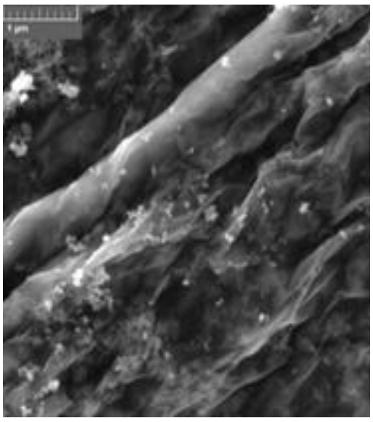

Fig.1. Scanning electron microscopy (SEM) image of FTGO603010 composite film

PO-21

Characteristics of Polymer Electrolyte Membrane Impedance Analysis

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Polymer electrolyte membrane (PEM) is the key component in modern fuel cell technology. Reduced fuel cell costs will make transition to sustainable energy faster and increase availability. Fuel cell is converting the chemical energy into electrical and the main role of PEM is a proton transfer, which can be characterised by proton conductivity [1]. In this work, the sulfonated poly (ether ether ketone) (SPEEK) based membranes are studied. The proton conductivity was measured using a simple differential cell method with copper electrodes as a current colletors and two Nafion membranes [2].

The method showed good correlation with existing data and it is also important to notice that the membrane surface is not damaged during impeadnce measurements using this method as it was shown by scanning electron microscope (SEM). Also, there is a reduction of cost of measurement because copper electrodes were used instead of platinum electrodes, which might be needed otherwise in a corrosive environment. Proton conductivity of SPEEK membrane depends on degree of sulfonation as it is shown on Fig. 1 (RH = 100%, 298K).

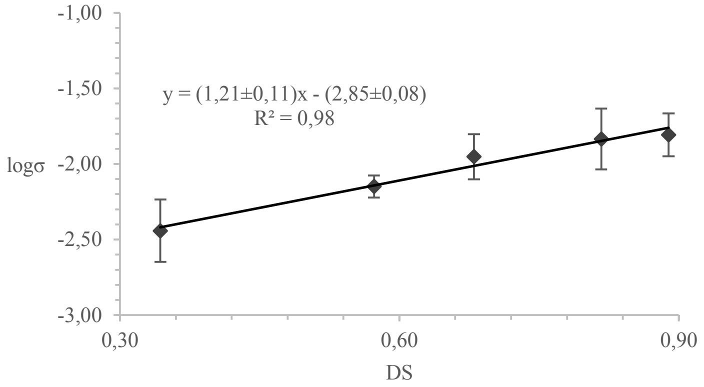

Fig. 1 The proton conductivity of SPEEK membranes (in S/cm) with different degrees of sulfonation DS.

Funding from European Union`s Horizon 2020 Research and Innovation Programme project under grant agreement No 768789 is greatly acknowledged.

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PO-22

Photo-catalytic and Electro-catalytic CO_2 Reformation – Reactions and Efficiencies in Separate and Combined Processes (Review)

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Energy harvesting with lowest environmental impact is one of key elements for cleaner future. Photocatalytic as well as electrocatalytic CO_2 reformation processes are considered as prominent methods. Thus, extensive research of CO_2 reformation is being done to find the right materials that inhibits crucial qualities. For photocatalysis that includes pronounced separation of light-generated opposite sign charge carriers, sensitivity to visible light, high quantum yield. As for elecrocatalysis, high CO_2 adsorption, chemical stability, multielectron reaction catalysts are necessary. Additionally, materials participating in the reaction process must provide with charge carriers at proper reduction and oxidation potentials.

To meet the set goal of lowering environmental impact and lower CO_2 amounts exhausted into the atmosphere by human activities, it is necessary to find right technology for capturing, storing, and reusing carbon dioxide. Various technologies and materials in different TRL are available and under development. Such as CuO loaded TiO_2 nanotubes for photocatalytic reformation [1], electrocatalytic reduction on copper [2,3]. Not only the prove of principle is necessary but estimation and more importantly determination of the efficiency of both electro and photo catalytic reformation of CO_2. In this work review of reactions and efficiency of both processes based on existing established technological methods is done. Additionally to side by side comparison a combined process of CO_2 reformation and its efficiency is investigated.

Acknowledgement: Funding from European Union`s Horizon 2020 Research and Innovation Program project under grant agreement No 768789 is greatly acknowledged.

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PO-23

Ternary Nafion©-graphene-Cu Composite for Electrochemical Reduction of CO_2 to Ethylene

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The use of carbon dioxide (CO_2) in chemical reactions is well-known, but in the recent years more and more attention is paid to this topic since it promises possibility to reduce CO2 amount in atmosphere and produce needed chemicals putting fossil resources in peace. Ethylene production is one of the possible compounds that could be produced from carbon dioxide; it is broadly used in synthesis of plastics and demand is growing [1]. The synthesis reaction is quite simple, but one of the problems is that specially chosen catalyst is needed to produce ethylene and reduce or avoid reactions that produce other compounds, e.g. formic acid. Because of the above mentioned reasons ethylene production could partially solve both carbon dioxide utilization and ethylene production problems, but some more research is needed to achieve this goal and new materials are needed, that could be used in production.

In our work ternary composite from graphene and copper and Nafion© that bounds catalyst to proton conductive membrane is synthesized and tested. Copper is known catalyst for production of hydrocarbons from carbon dioxide including ethylene. Graphene has several properties such as high surface area, conductivity and mechanical stability that are necessary for catalyst support [2]. Nafion© is well-known proton conductive polymer, that in this case potentially improves contact with membrane, since our goal is to prepare material that would be suitable for ethylene production and could be coated on Nafion© proton conductive membrane by combining these materials with polymer.

Acknowledgement: Funding from European Union`s Horizon 2020 Research and Innovation Program project under grant agreement No 768789 is greatly acknowledged.

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PO-24

1,3-Dimethylimidazolium Dimethyl Phosphate and SPEEK based Composite Proton Conducting Membranes

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Important part of fuel cells is polymer electrolyte membrane(PEM) or otherwise known as proton exchange membrane. PEM main function is to evade direct contact between air and fuel and also to ensure the proton transfer. Ionic liquids are suitable for improving the proton transfer at higher temperatures and improving mechanical properties of membranes [1,2]. In this work, the sulfonated poly (ether ether ketone) (SPEEK) membrane composite with ionic liquid [MMIM][DMP] (1,3-dimethylimidazolium dimethyl phosphate) have been studied. Ionic liquid structure is shown in Fig. 1. The proton conductivity was measured at different percentages of ionic liquid and degrees of sulfonation for membranes. The degree of sulfonation was obtained by widely used titration method [3].

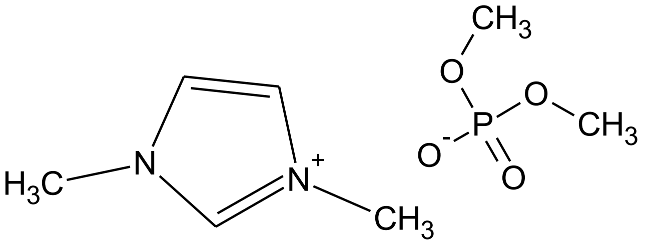

Fig.1 1,3-dimethylimidazolium dimethyl phosphate structure.

Autolab potentiostat/galvanostat PGSTAT302 was used for impedance measurements in a frequency range from 1 to 50 kHz (10 mV signal amplitude). The differential measuring cell was used as a sample holder and commercial NAFION membrane as a reference.

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PO-25

Nanostructured Nitrogenated Carbon Materials as Promoters in Hydrogen Energy Technologies

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Hydrogen in the Earth can not be found in free form as a gas because the gravitational force of the Earth can not sustain it, therefore extensive research into new materials and technologies to produce hydrogen from renewable sources is being conducted. Hydrogen as an energy carrier in modern technology is irreplaceable in emission-free transport and independent energy supply. With the development of nanotechnologies, the synthesis and research of various forms of carbon nanostructures increased rapidly in the 1980s. The first uses of activated carbon as a carry of catalyst, especially platinum, were applied in various industrial processes, both in the food industry and in the chemical industry and energy technologies - energy harvesting and storage. Cheap, productive and stable catalysts that replace platinum in hydrogen technologies are needed for hydrogen production (water splitting with light or electricity), storage (hydrogen bonding in solids or on the surface) and for use in energy production (microbial and proton exchange membrane fuel cells).

In 2010, nitrogen-modified graphene (N-graphene) has been shown to have better electrocatalytic activity, long-term activity, and stability against impurities in oxygen reduction in alkaline fuel cells, as it was previously shown for N-carbon nanotubes. Theoretical calculations and experimental results show that the direct four-electron process, which is maximally favorable for the oxygen reduction reaction, takes place on energy-stable and practically-derived materials as Fe and N-doped graphene. Carbon-nitrogen bond is one of the most common in nature, this strong covalent bond is the basis of many compounds in organic chemistry and biochemistry. In our work, the main challenge is to develop a methodology for the self-extracted nanostructured carbon materials (multi-layer graphite and alkaline activated charcoal) for nitrogen-doping. Functionalization with nitrogen atoms is also possible by exfoliation in various water-based electrolytes, such as ethyl ammonium nitrate, ammonium nitrate, ammonium sulfate and sodium nitrate.

PO-26

Gas Separation Using WO_3/NiOOH red-ox Mediator Pair in Four Electrode, Dual Chamber Electrolysis Cell

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So far a four electrode dual-chamber cell setup, has been studied for the purpose of hydrogen and oxygen gas separation in water electrolysis. The idea is based on the red-ox mediator electron bridge, connecting the anode and cathode space. So far a NiOH/$Ni(OH)_2$ electrode mediator pair has been investigated, where anode and NiOOH electrode are placed in the anode space and cathode together with $Ni(OH)_2$ electrode, in cathode space. Both chambers are hermetically separated and electrical potential is applied to the cathode and anode. During the process, cathode and anode work as in typical two electrode electrochemical cell, but NiOOH electrode accumulates H ions and $Ni(OH)_2$ loses H ions, which results in electron transfer between the cathode and anode space through the mediator circuit [1, 2].

In this work, the electrochemical properties of NiOH/$Ni(OH)_2$ and WO_3 / H_xWO_3 red-ox mediator pair electrodes are studied. The electrodes were prepared using magnetron sputtering method, where ITO coated glass was used as substrate. After the electrode synthesis, their voltammetric curves were obtained, by placing the electrodes in a four electrode, two-chamber electrochemical cell. In NiOOH/$Ni(OH)_2$ electrode case, 1M KOH solution was used as the electrolyte, while 0.5M H_2SO_4 solution in the case of a WO_3 / H_xWO_3 electrode pair.

It was found that using NiOOH/$Ni(OH)_2$ mediator pair, process is significantly limited by the conductivity of $Ni(OH)_2$ layer, and in WO_3/H_xWO_3 pair case, by WO_3 layer. Knowing that the oxygen evolution reaction takes place more actively in alkaline solution and hydrogen evolution reaction in acidic, also electrochemical activity was measured in the configuration of NiOOH/H_xWO_3 mediator pair mix. In this setup, the anode space contained alkaline and cathode space acidic solutions. The Voltammetric measurements of this setup revealed that the current at 3.5V potential, between the electrodes was 100 times higher, as with NiOOH/$Ni(OH)_2$ and WO_3/H_xWO_3 electrode configurations.

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PO-27

Nanomaterials and Key Technologies for Bio-H_2 Separation

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Hydrogen is an energy carrier and clean fuel because the only product of its combustion is water. Therefore hydrogen is considered as the only real candidate for the replacement of fossil resources, and energy saver & fuel of the future. Biological natural systems that evolve hydrogen are categorized into four primary groups [1]: water-splitting photosynthesis; photofermentation; dark fermentation; and microbial electrolysis processing (Fig. 1).

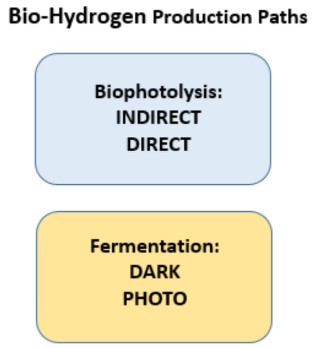

Fig.1 Schematic representation of the primary biological routes [1].

In our research [2] we found that hydrogen produced in dark fermentation process is required to remove continuously, in order to proceed with the release of hydrogen with no reduced intensity. Higher concentrations of dissolved hydrogen in substrate of bioreactor appears to inhibit the hydrogen production, and more by-products such as ethanol, butanol, lactate, and acetone is generating [3]. Therefore separation of biohydrogen from substrate solution and headspace gas in reactor is essential for sustained the biohydrogen production process, and treatment from sulphur and ammonia contamination is necessary for the hydrogen utilization in fuel cell. For hydrogen removal from substrate solution mixing or bubbling with neitral gas are used, we suggested the reactor walls make transparent to hydrogen by making them of nano-porous material, where the pores are peeled off with a hydride-forming metal or alloy [2]. Many technologies have been applied for hydrogen separation from headspace gas in reactor, such as pressure swing adsorption, solvent adsorption, cryogenic recovery and membrane [3]. The separation and selective purification of hydrogen via membrane technology appear to be promising because there exist many types of organic and inorganic membranes to enrich hydrogen, which can be subdivided into porous or non-porous membrane.

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PO-28

The Impact of Zirconium Phosphate Content on Proton Conductivity of Composite Polymer Electrolyte

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Great effort has been made to increase the proton conductivity of various proton exchange membranes (PEM), to find an alternative to the commonly used Nafion® PEM. The sulfonated poly(ether ether ketone) (SPEEK) is widely accepted as a potentially suitable replacement material in PEM. By combining it with various filler materials (such as Ionic liquids (ILs)) to form composites, the conductivity values of SPEEK can reach up to 0,1 S/cm [1]. SPEEK/IL composites possess high proton conductivity even in absence of water, especially at temperatures above 100 °C [2]. However, the addition of IL deteriorates mechanical properties of the resulting composite since IL acts as a strong plasticizer due to its large molecular size. Thus a partial replacement of the IL with an ion conducting material that have less impact on structural strength of the polymer should be considered. As an additive, zirconium phosphate (ZrP) is known for enhancing proton conductivity as well as mechanical properties which makes it a good candidate as a filler component in polymer electrolyte [3,4].

Two sets of samples of composite membranes were prepared in 1:4 and 1:8 IL/SPEEK wt. ratio. For each set, four samples were prepared with added ZrP/SPEEK wt. ratio ranging from 0,125:4 to 1:4. Conductivity measurements were done using closed bipolar measurement cell with controllable temperature and atmosphere. Conductivity as a function of ZrP content for different IL/SPEEK composites is discussed and suitability of ZrP as additive to IL/SPEEK composites evaluated.

Funding from European Union's Horizon 2020 Research and Innovation Programme project under grant agreement No 768789 is greatly acknowledged.

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PO-29

Preparation of ZnO Modified TiO_2 Nanoporous Coatings and Their Photocatalytic Properties

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TiO_2 photocatalysis is widely used in a variety of applications and products in the environmental and energy fields. Various techniques had been widely applied to remove different types of toxic organic enviromental pollutants from waste water by using methods of adsorption and degradation. One of the most promising and cost efficiently way to do it is in presence of photocatalysts and sunlight [1]. Due to its wide band gap (3.2eV) pure TiO_2 anatase as photocatalyst can be used only under UV irradiation. As only about 5% of sunlight that reaches the Earth contains UV irradiation modification of TiO_2 structure is required. By increasing the specific surface area and modification with various dopants efficiency of TiO_2 photocatalysts in VIS irradiation can be improved dramatically [2]. As ZnO is well known photocatalyst with high activity in visible light as dopant it could improve light adsorption properties of TiO_2 and decrease the band gap of it.

In the present work formation of active nanoporous TiO_2 photocatalysts and their modification with ZnO were studied.

TiO_2 nanoporous coatings on Ti foil with surface area $100cm^2$ were prepared by using plasma electrolytic oxidation (PEO) method in 0.5M H_2SO_4 electrolyte and by using 160V DC voltage. For modification of TiO_2 coatings with ZnO spray pyrolysis method where used. After preparation samples were dried and calcined at 400^oC for 2h in air.

Photocatalytic properties of obtained samples were tested by using degradation method of methylene blue (MB) solution under UV and VIS light illumination. Degradation rate of MB were measured by using spectrophotometer. From obtained results reaction constant (k) in the pseudo first order reaction were calculated.

As prepared ZnO modified TiO_2 nanoporous coating photocatalysts are with higher photocatalytic activity with respect to pure TiO_2 nanoporous coating photocatalyst.

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PO-30

Photonic Sensor for Distinguishing Dead and Alive Bacteria Content for Monitoring of Decontamination Efficiency

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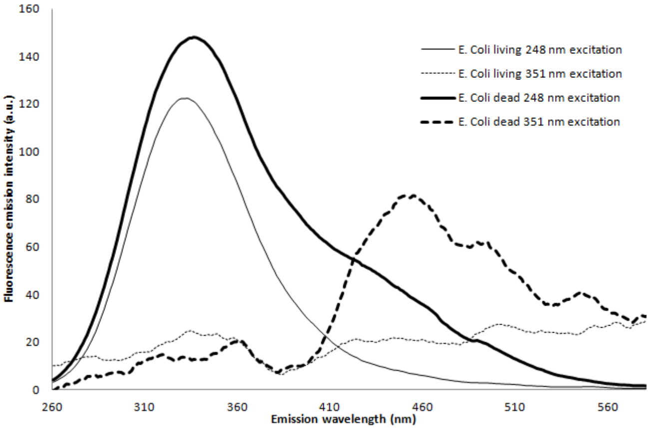

Fig 1. Laser induced fluorescence (LIF) spectra of dead and living bacteria, excited by laser radiation at 248 nm and 351 nm. A study was performed within the FP7 EDEN project. The dashed lines are for 351 nm and solid lines for 248 nm excitation, respectively. One can see a fluorescence peak at ~460 nm due to the emission of the dead bacteria.

The aim of the study was to develop a prototype of photonic sensor, which enables detection of bacteria and distinguishing between live and dead bacteria in indoor environment setting (e.g., in bio-laboratories, hospitals, emergency vehicles, etc.) to control the decontamination efficiency without applying any marker chemicals, but only using the autofluorescence of the bacteria. It has been revealed from our previous studies that there is a spectral difference between living and dead bacteria, but so far no-one has paid enough attention to exploit research findings in that field in sensoric applications. The sensor was designed to detect bacteria on the surfaces in non-contact mode. Our research revealed how to differentiate between emission spectra of living indicator bacteria from the dead ones in various environments-to-be-decontaminated by using different autofluorescence excitation and emission wavelength combinations (see Fig. 1 comparing various LIF spectra). Experiments were performed to find the lowest detectable concentration of living bacteria on the test plate and to clarify the residual amount of decontamination treatment, which is needed after the photonic indicator no longer detects living bacteria. In-field experiments were carried out showing how to compare the bacterial death probability indication from the sensor prototype with the results of 1-week agar-growth colony based on standard counting methods. The basic principles and challenges in creating such photonic sensors will be discussed.

PO-31

Defects Creation in Undoped and Ce - doped $Gd_3(Ga,Al)_5O_{12}$ Crystals Under Irradiation in the Gd^{3+} - related Absorption Bands

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Single crystals of $Gd_3(Ga,Al)_5O_{12}$:Ce are intensively studied as promising scintillator materials for medical imaging because of their extremely high light yield (close to 60 000 ph/MeV), excellent energy resolution (4.2%@662 keV), relatively high density (6.63 g/cm^3), fast scintillation response, high radiation stability, and high hardness [1-2]). The gadolinium sublattice is known to play an important role in the energy transfer from the host to Ce^{3+} ions owing to an effective excitation energy migration along Gd^{3+} ions terminated by the nonradiative Gd^{3+} - Ce^{3+} energy transfer (see, e.g., [3] and references therein).

We have found that under excitation of the undoped and Ce - doped $Gd_3(Ga,Al)_5O_{12}$ crystals at 85 K in the Gd^{3+} absorption bands, arising from the $^8S_{7/2} – {}^6I_J$ and the $^8S_{7/2} – {}^6P_J$ electronic transitions of Gd^{3+} ions, not only the Gd^{3+} - related $^6P_{7/2}$ - $^8S_{7/2}$ luminescence, energy migration along Gd^{3+} ions, and energy transfer from Gd^{3+} to acceptors (intrinsic defects or Ce^{3+} ions) resulting in their excitation can take place [3], but also stable intrinsic electron centers are effectively created. This is evident from the appearance of the thermally stimulated luminescence (TSL) glow curve peaks at about 120 K and 250-270 K whose creation spectra correlate with the Gd^{3+} absorption spectrum. The electron centers can appear as a result of electrons release from the excited states of the acceptors and their subsequent trapping at the intrinsic defects responsible for the TSL peaks. In case of $Gd_3(Ga,Al)_5O_{12}$:Ce, the Gd^{3+} – Ce^{3+} energy transfer results in the Ce^{3+} luminescence and release of electrons from the $5d_2$ excited state of Ce^{3+} into the conduction band. As much as we know, this is the first observation of defects creation under irradiation in the Gd^{3+} - related absorption bands.

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PO-32

EPR Spectroscopy of Mn^{4+} Doped Germanium Garnet

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In recent years, Mn^{4+} doped fluorides and oxides have gained a lot of attention [1,2] as these materials can provide narrow-band red emission needed for next-generation warm white LEDs, which provide radiation similar to thermal light sources and are perceived as cozy by humans. The local geometry and chemical environment strongly influences the emission wavelength of the Mn^{4+} ion. Therefore, electron paramagnetic resonance spectroscopy is an excellent tool to reveal such centre properties. The aim of the present study is to characterize the paramagnetic Mn centres in the inverse germanium garnet, which has been considered as red emitter for high-power phosphor-converted LED applications [3].

The germanium garnet phosphors $Y_2Mg_{2.97}Li_{0.02}Ge_3O_{12}$ doped with Mn^{4+} ions of 0.01, 0.05 and 0.5 mol-% concentrations were synthesized by sol-gel method. The EPR experiments were carried out with a Bruker CW X-band spectrometer at T = 4 - 300 K. The Xepr software provided by Bruker and the EasySpin analysis package [4] were applied in data analysis. It is commonly supposed that the Mn^{4+} ions substitute cations in the octahedral coordination, i.e. Mg^{2+} ions in this garnet. In the sample with low Mn concentration the EPR spectra revealed that Mn^{4+} ions are situated in a high symmetry site corresponding to the octahedral coordination as expected. For higher Mn concentrations the spectra become more complex with broadened EPR lines. The revealed features allow to identify multiple centres, distortions in the crystal lattice near Mn ions and possible effects due to the manganese pair formation. The local geometry of the observed entities and the variation of the values of EPR parameters depending on the Mn concentration will be presented. Finally, the influence of low and high Mn doping on formation of the EPR active centres will be discussed.

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PO-33

Pressure-induced Structural Changes in α-MoO_3 Probed by X-ray Absorption Spectroscopy

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After the discovery of graphene, other members of 2D materials family, including molybdenum trioxide (α-MoO_3), have been intensively investigated due to their unique properties. Orthorhombic α-MoO_3 (space group *Pbnm*) is thermodynamically stable at ambient conditions and has an anisotropic layered structure stabilized by van der Waals forces [1].

According to X-ray powder diffraction and Raman spectroscopy studies [2], α-MoO_3 transforms under pressure to monoclinic MoO_3-II phase ($P2_1$/m) at ~12 GPa and to monoclinic MoO_3-III phase ($P2_1$/c) at ~25 GPa. In this study, we conducted pressure-dependent X-ray absorption spectroscopy measurements of α-MoO_3 up to ~36 GPa to study pressure-induced changes in its local atomic structure. We found that smooth variation of the Mo K-edge XANES occurs up to ~26 GPa due to gradual decrease of the interlayer spacing, whereas the XANES changes abruptly at higher pressures (Fig. 1) due to a collapse of the layers leading to oxide structure reconstruction. To extract the detailed information on this process, the EXAFS analysis beyond the first coordination shell of molybdenum was performed using reverse Monte Carlo calculations [3] and allowed us to build a structural model consistent with the experimental data.

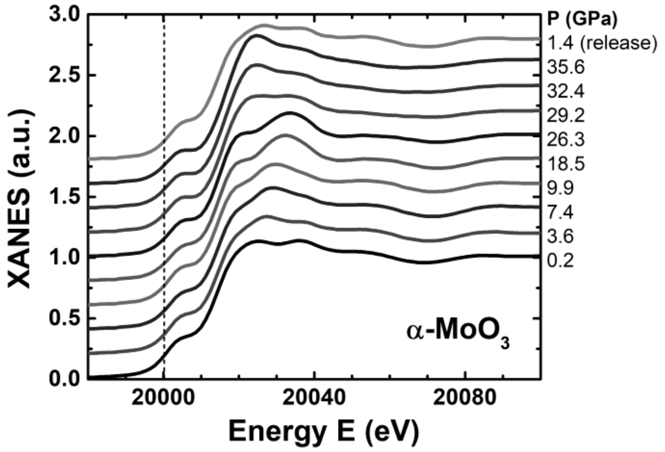

Fig. 1 Pressure dependence of the Mo K-edge X-ray absorption near edge structure (XANES) in α-MoO_3.

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PO-34

Raman Spectroscopy Studies of Temperature Dependent Ferroelectric Instability in $SrTi_{18}O_3$

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Strontium titanate is a model quantum paraelectric in which, in the region of dominating quantum statistics, the ferroelectric (FE) instability is inhibited due to nearly complete compensation of the harmonic contribution into ferroelectric soft mode frequency by the zero- point motion contribution. The enhancement of atomic masses by the substitution of ^{16}O with ^{18}O decreases the zero-point atomic motion, and low-T ferroelectricity in $SrTi^{18}O_3$ is realised [1]. In this study, we report on temperature dependent (T = 10 - 300K) Raman spectra measurements in $SrTiO_3$ and $SrTi^{18}O_3$.

We have identified modes (e.g. 171 and 519 cm^{-1}) correlated with FE phase, as well as modes (e.g. 145 and 422 cm^{-1}) associated with tetragonal phase. As x-ray diffraction studies does not detect any structural changes in FE phase [1], and x-ray absorption studies [2, 3] reveal that the local structure of the Ti is the same in whole temperature range (10 - 300K), we suggest that $SrTi^{18}O_3$ as an example of dynamic FE phase transition, where average structure does not change, but the relative movement of the ions is strongly correlated, and this correlation (e.g. of Ti-Ti chains) is responsible for macroscopic FE phase. This suggestion is supported by the theory of formation of lower symmetry dynamical clusters in [4].

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PO-35

Depth Profiles of Damage in MgO Single Crystals Irradiated with Swift Heavy Ions

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MgO is a promising material for applications in high-energy and nuclear technologies due to its high radiation and heat resistance. The effect of irradiation with GeV energy heavy ions on structure, dislocation mobility and hardness of MgO single crystals was investigated. The crystals were irradiated at the UNILAC of GSI, Darmstadt with U, Au and Bi ions at fluences 5×10^{11} – 7×10^{13} ions/cm^2. The methods of nanoindentation, dislocation mobility and chemical etching, which are sensitive to ion-induced dislocations and other extended defects, were used. In irradiated samples XRD shows a single-crystalline state with radiation-induced disordering. Chemical etching reveals ion-induced dislocations. The accumulation of dislocations leads to substantial decrease of dislocation mobility and moderate increase of hardness in irradiated crystals. However, the effects in MgO are markedly lower in comparison with those observed for radiation-sensitive materials, such as LiF. The depth behavior of ion-induced effects in dislocation mobility and hardness correlates with the change of calculated electronic energy loss. The ion-induced hardening as a function of average absorbed energy (E_a) for investigated heavy ions was compared with the results reported in [1] for light Kr and N ions. At $E_a > 2\times 10^{24}$ eV/cm^3, the hardening effect in both cases turns to saturation. However, heavy ions create stronger hardening at saturation (around 37% against virgin MgO) than light projectiles (24 %). For the latter, a notable contribution of nuclear energy loss to hardening in the end-of-range region above $E_a > 10^{26}$ eV/cm^3 is observed. In general, the results confirm the high resistance of MgO to irradiation with swift heavy ions. MgO crystals irradiated with doses up to 950 MGy exhibit improved hardness and maintain a single-crystalline state, integrity and micro- plasticity at indentation.

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PO-36

Effect of In on the ZnO Powders Morphology and Microstructure Evolution of ZnO:In Ceramics as a Material for Scintillators

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ZnO:In as transparent ceramics are of interest for use as fast scintillators with high efficiency [1]. This requires high intensity of X-ray- or photoluminescence (PL) exciton peak, negligible defect-associated ("green") PL, short decay time and high hardness without grain boundaries (GBs) brittleness. For ensuring such properties, a high-quality microstructure should be formed, which in turn depends on adhesion processes on the powders contact, behavior of grain boundaries (GBs) and diffusion activity during sintering [2].

In this work we consider the influence of shape, surface faceting of the original and In-doped ZnO powders on the microstructure formation, optical and mechanical properties of undoped and In (0.13 wt. %) doped ZnO ceramics. All ceramics obtained by hot pressing at 1100 ^{0}C have been investigated using nanoindentation, SEM, TEM and PL methods.

It was found that during the powder mixing indium facilitates a transition of initially faceted ZnO particles to rounded, promoting good sintering with formation of diffusion active high-angle GBs. Sintered ZnO:In ceramics show improved microstructure, including fine grains, faceted GBs with In and Zn access, and absence GBs brittleness. Such modifications of GBs provide reliable ways to remove point defects, reduce the I_{def}/I_{exc} parameter for PL by 15 times, for X-ray luminescence by 85 times with decay time of about 1.1ns. Results characterize ZnO:In ceramics with improved GBs properties as a prospective material for fast scintillators.

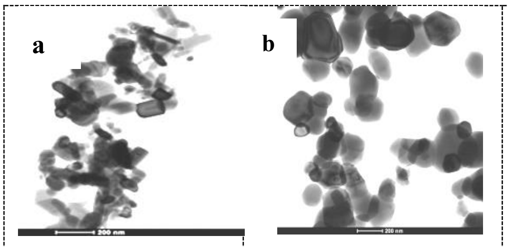

Fig.1 TEM images of initial ZnO powder (a) and doped ZnO:In (b) powder prepared by mixing at room-temperature

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PO-37

Vibrational Spectra and Lattice Dynamics in the β Form of White Phosphorus

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White phosphorus is a molecular crystal whose structural elements are P_4 tetrahedral molecules. At present, 3 polymorphic modifications of white phosphorus α, β and γ forms are known. In this paper we investigated the low temperature β form of white phosphorus by the methods of vibrational spectroscopy. The tetrahedral molecule P_4 has 3 internal vibrations of classes A_1, E and F_2. All three vibrations are active in Raman spectra, but only F_2 is active in IR spectra. Experimentally in β form we observed all three vibrations in both the IR and Raman spectra. In both the IR and Raman spectra, the vibration $\nu_3(F_2)$ is splitting by not less than 8 components, and the vibration $\nu_2(E)$ by 6 components. The band $\nu_1(A_1)$ in the IR spectrum is splitting into a doublet, and a narrow single band is observed in the Raman spectrum. The discrepancy between the positions of the bands in IR and Raman spectra indicates the existence of an alternative prohibition. This means that the unit cell in the β form is centrosymmetric For vibrations $\nu_2(E)$ and $\nu_3(F_2)$, the distance between the extreme components of the multiplet exceeds 16 cm^{-1}, and the total number of observed bands for $\nu_2(E)$ (taking into account the IR and Raman discrepancy) is 11, and for $\nu_3(F_2)$ is 15.

The structure of the β form has $P\overline{1}$ (No. 2) space goup containing six P_4 molecules per unit cell [1]. The three internal vibrations A_1+E+F_2 of the P_4 molecule in the β crystal form are represented as: $A_1 = 3A_g+3A_u$, $E = 6A_g+6A_u$ and $F_2 = 9A_g+9A_u$. Vibrations A_g are Raman active and vibrations A_u are IR active. The splitting of internal vibrations of the molecule P_4 in the crystal does not exceed 20 cm^{-1}. The vibrations of the lattice and librations of the P_4 molecules correspond to the symmetries $18A_g+15A_u$ and are located in the low frequency region 20-120 cm^{-1}.

Ab initio calculations have been performed by using hybrid exchange densitu functional theory to determine equilubrium geometryie of crystal lattice and phonon frequencies. The Grimme dispersion correction for energy and gradient has been used in combination with B3LYP functional. CRYSTAL14 computer code was used.

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PO-38

Float Zone Single Crystals for Testing Rods, Pulled Under Electron Beam Heating

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KEPP EU developed new method of archiving silicon rods for future application for growing FZ single crystals under electron beam heating (EB rods). Main requirements to such rods are purity, stable required geometry and mechanical strength. The purity of main impurities as boron and phosphorus must be less 10 ppta. Control of purity on this level in silicon possible by FTIR Spectroscopy at He temperature, only. By other side, technology of EB rods came to rods diameter 300 mm [1]. FZ technology to 300 mm FZ single crystals is absent.

Target of our current activity is developing FZ method of silicon single crystal growth by pedestal technique. In present paper described results of activity in mathematical modeling of process, practical implementation. Inductor shape in the mathematical model was optimized to maximize melt height and therefore reduce the risk of melt center freezing. As results the possibility of using high-frequency generators with a power frequency of less than 2 MHz is established in such processes.

The conformity of the primary model and practical results is analyzed. The properties of grown single crystals of silicon have been studied and their compliance with modern requirements for such single crystals has been analyzed. The results are discussed.

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PO-39

Production of Phosphorescent Coatings Using Plasma Electrolytic Oxidation Method

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Plasma electrolytic oxidation (PEO) is a process which allows to create ceramic oxide coatings on metal surfaces. The coatings have increased hardness as well as outstanding resistance to corrosion and wear when compared to an unprocessed metal surface. In a relatively short amount of time it is possible to produce tens of micrometres thick oxide layer as well as to modify its crystalline structure, morphology and composition by changing PEO process parameters. During the recent years, a selection of luminescent PEO coatings have been developed by using certain elements in the preparation. To be feasible for industrial applications the method still has to undergo many developments to improve efficiency of the process and reproducibility.

The coatings were developed on industrially pure aluminium substrate. The main goal of this research was optimization of PEO process parameters to improve luminescence properties, afterglow duration and intensity of the acquired phosphorescent coatings. The main focus was on the effects of additive concentrations used in electrolyte, duration of the process and impact of electrical parameters. The optical properties of the acquired coatings were studied using photoluminescence, thermally stimulated luminescence (TSL) and luminescence decay kinetics measurements. Energy dispersive x-ray fluorescence spectroscopy (EDX) was used to determine the chemical composition of coatings to make further improvements to electrolyte and process. SEM images were taken to study morphology of the coatings.

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PO-40

Permittivity Increase of Carbon Black/Silicone Oil Suspension Induced by Electric Field

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A direct current (DC) electric field increases electrical conductivity of the carbon black/silicone oil (CB/SO) suspension by five orders of magnitude [1]. In our current study, the DC electric field induced permittivity change of the suspension was researched. The CB/SO suspension containing 0.2 wt% (concentration far below permittivity percolation threshold) of the CB filler was used for the experiments. It was found that application of the DC field to the suspension, simultaneously with the conductivity increase, results in the permittivity increase by up to three orders of magnitude in case of high field strengths (Fig.1). The permittivity increase of the suspension is due to the alignment of initially randomly positioned CB particle aggregates, which form a network of branched structure of micro-capacitor chains and densify upon increasing electric field strength and time.

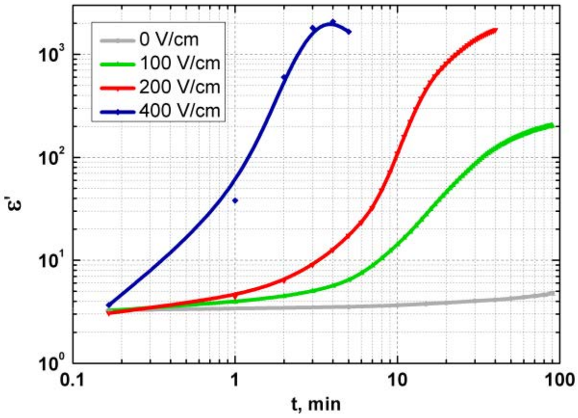

Fig.1 Relative permittivity (at 1 kHz) versus time for the CB/SO suspension containing 0.2 wt% of the CB depending on the DC field strength.

The obtained results can be used in development of polymer/nanoparticle composites with anisotropic properties.

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PO-41

Determination of Molecular Structure of Schiff Base Complexes with Cu Ions

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Schiff bases as well as coumarin derivatives are known for having a broad spectrum of biological activity. They form stable complexes with transition metal ions often showing an increase in biological activity, what makes them perfect as potential pharmacological agents. The potential of pharmacological action depends on the chemical structure, therefore, the binding mechanism between copper ions and organic ligands in biologically active Schiff base complexes with 7-hydroxycoumarin derivatives has been studied. [1, 2]

To get structural information about non-crystalline coumarin Schiff base complexes with copper ions the multi-approach methodology has been applied. Using the XAS (X-ray absorption spectroscopy) technique the local atomic environment around the specific element can be described. EXAFS and XANES spectra have been measured at the XAFS beamline (Elettra-Sincrotrone Trieste, Italy). As a support for structural characterization, several spectroscopic as well as analytical techniques, i.e. FTIR spectroscopy, elemental analysis, DFT calculations, have been applied. [3, 4]

Combination of mentioned experimental methods enabled to obtain information about coordination site of studied complexes. With EXAFS analysis a local atomic environment of copper ions have been determined i.e. the number and type of neighboring atoms, as well as their average distance to Cu ion have been found what allowed to describe the molecular structure of the studied Schiff base complexes.

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PO-42

Effect of Composition of Steel and Holding Time on the GB Wetting by Copper

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Brazing is the physico-mechanical joining in which braze is melted to form the joint between subsequent substrates. The effectiveness of joint formed and its reliability is of prime importance in today's electronics and electronic packaging systems. These issues have been dealt by the scientific community over the years precise solutions have been formulated. There is however one prevalent issue in the industry which still needs to be understood and solved, the problem of grain boundary wetting followed by grain boundary penetration. Grain Boundary wetting is often required at the joint interface for successful joint formation. But this also leads to penetration of grain boundaries by liquid braze which forms a liquid condensate network. This network in the long run leads to failure of the joint by forming separated grain boundary crystals at the interface. In this experiment, five different steels of varying Cr composition are taken and carried out brazing with pure Cu foil under inert gas (Ar) environment. The main focus was on the microstructure characterization and the measurement of grain boundary penetration. The emphasis was also kept on the behavior of braze with steels as function of varying Chromium (Cr) composition.

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PO-43

Deuterium Concentration's in Austenitic Stainless Steel by Deuterium Irradiation. Effects Temperature Irradiation

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The kinetics of structural transformation development in the austenitic stainless steel was traced from deuterium thermodesorption spectra, TEM as a function of deuterium concentration and temperatures irradiation. The samples were pre-implanted with 12 keV deuterium ions in the dose range from 8×10^{14} to 2.7×10^{18} D/cm^2 at the different irradiation temperatures: 100, 240, 295, 380, 420 and 600 K.

Temperature 100 K. The maximum attainable concentration of deuterium in steel is C=1 (at.D/at.met.=1/1). At C≥0.5, two hydride phases are formed in the steel, the decay temperatures of which are 240 K and 275 K. The hydride phases are formed in the bcc structure resulting from the martensitic structural transformation in steel [1].

Temperature 295 K. The medium-dose region is characterized by radiationinduced action on the steel in the presence of hydrogen. The process results in the formation of the energy-stable crystalline nanostructure of steel, having a developed network of intercrystalline boundaries. The basis for this developed network of intercrystalline boundaries is provided by the amorphous state. The total concentration of the accumulated deuterium in the region of medium implantation doses makes 7 to 8 at.% [2].

Temperature 380; 420; 600 K. In a deuterium thermodesorption spectras the extended area desorption deuterium in a range of temperatures 450-900 K, caused by formation of local structural in radiationinduced a layer is observed. Formation of local structural can be caused a segregation a steel component, in the course of implantation deuterium (radiating influence local structural at presence deuterium). The total concentration of the accumulated deuterium in the region of medium implantation doses makes 1 to 3 at.%.

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PO-44

Temperature Range of Helium Retention From Austenitic Stainless Steel Implanted Helium at 600 K

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Helium thermal desorption spectra were investigated on the samples of austenitic steel 18Cr10NiTi pre-implanted with 24 keV helium ions at current density 5 μA/cm^2 in the dose range from 5×10^{16} to 4 × 1018 He/cm^2 at the sample temperature Tirr ~ 600 K.

The spectrum of helium thermodesorption from the samples exposed to doses ~ 5×10^{16} He/cm^2 represents the temperature-scale smeared region of helium desorption with maxima in the temperature ~1470 K.

The increase in a dose of the implanted helium is accompanied by advancement of a spectrum of allocation of helium in a direction of fall of temperature. For a dose 4×10^{16} He/cм^2 the spectrum helium thermodesorption represents to the area washed away on a temperature scale desorption with badly divided peaks in a range of temperatures 1000 – 1400 K.

At the further increase in a dose of the implanted helium there is a qualitative change of a spectrum thermodesorption the helium, shown in formation of peak to maximum temperature at Tm ~ 1000 K. The further increase in a dose of the implanted helium leads to growth of intensity of this peak of a spectrum thermodesorption and it becomes prevailing.

Proceeding from representation that atoms of helium in a crystal lattice of a steel form vacancy – helium complexes, peak with temperature of a maximum ~1000 K corresponds to temperature of disintegration of such complexes. Thus the quantity of atoms of helium in a complex is strictly defined. Further energy of activation desorption helium will be calculated, the analysis of the received results of research is offered.

PO-45

Yttrium Oxyhydrides as a New Family of Mixed-anion Functional Materials

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We present our recent advances in the discovery and theoretical design of the yttrium oxyhydride (Y–H–O) systems. We consider the Y–H–O crystal chemistry, synthesis and characterization of both bulk powder and thin film samples, and discuss structural stability, electronic, elastic, vibrational and optical properties. The main fundamental aspect of our work is that we have shown that the degree of functionality of Y–H–O systems can be directly regulated via the oxygen/hydrogen ratio in the chemical composition. The interplay of different anions along with spontaneous lattice symmetry-breaking effects caused by the oxygen insertion represents the main focus of our strategy for prediction of novel mixed-anion materials with the stable lattice geometries and unusual structure-property relationships.

PO-46

Reorganization Energy Quality Tested by Statistics

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One of the quantities used for mobility calculations of charge carriers in organic semiconductors is the reorganization energy λ, straightforward calculations of which employ the ΔSCF scheme canonized by A. Klimkāns.[1] Density functional theory is a frequently used low-cost alternative for computationally-extensive post-SCF methods, and applicability of different density functionals for this is frequently explored.[2,3] At the same time, one of the factors not so frequently considered is the size and quality of the basis set. We hereby provide a systematic comparison of results with Pople basis sets with results by Møller–Plesset perturbation theory, obtained by various statistical methods which should mitigate the system-dependent error.[4] Instead of directly comparing the quantities of interest, we carry out this study on regression parameters for a series of 4'-substituted 2-benzylideneindane-1,3-diones.

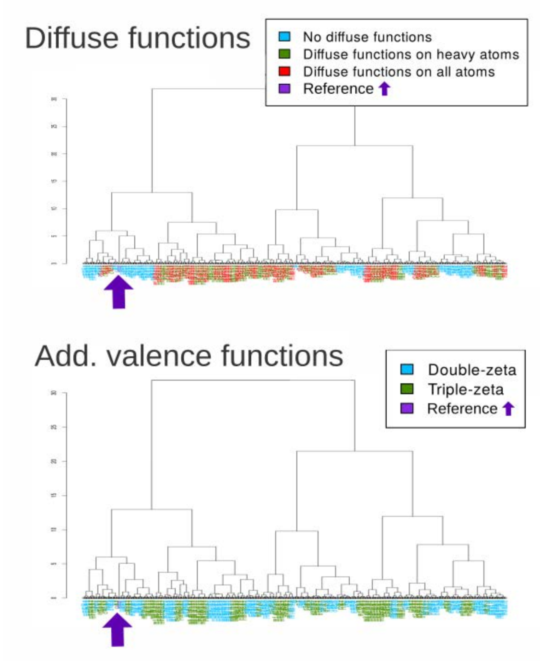

Fig.1 Hierarchical clustering analysis shows that employing diffuse functions in basis set actually worsens results, whereas using triple-zeta instead of double-zeta has virtually no effect.

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PO-47

Anisotropy of Singlet Oxygen Luminescence in Silica

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Oxygen molecules (O_2) are introduced in interstitial spaces of SiO_2 glass (silica) by high-energy irradiation or by manufacturing process. They are much studied because of the importance of silica as an optical material.

The 1st excited electronic state of O_2 ($^1\Delta_g$, the "singlet oxygen") plays a key role in cell photobiology, photosynthesis and photocatalysis [1]. In many solid and liquid matrices it gives rise to weak and highly forbidden a $^1\Delta_g \rightarrow X\ ^3\Sigma_g^-$ near-infrared ($\hbar\omega$=0.97eV) photoluminescence (PL) band. Its lifetime (τ) in silica (≈0.85s) is the longest reported for singlet O_2 in condensed matrices at 295K. The $X^3\Sigma_g^-$ ground state and $a^1\Delta_g$ excited states have non-zero magnetic moments, offering a perspective to detect O_2 by diamond-based nanosized magnetic field sensors [2].

The dynamics of O_2 motions in silica matrix is determined by the size of the nanovoids ("cages") in SiO_2 network. While O_2 diffusion in silica is well-studied, it is not known if O_2 can rotate in its cage in silica. We studied the polarization anisotropy of singlet oxygen (a→X) PL with excitation by linearly polarized light in the temperature range 300K-14K. The PL was unpolarized (P<1%) under excitation (λ=766nm) to the 2nd excited state ($X \rightarrow b^1\Sigma_g^+$). P did not increase at T=14K. In contrast, under a near-resonance excitation (λ=1064nm) to the 1st vibrational level ($X(v=0) \rightarrow {}^1\Delta_g$ (v'=1)) the PL had non-zero polarization degree (P=+2.5%) at T=295K which increased to +6.5% at 14K. The PL is extremely weakly allowed (τ≈1.15s at 14K) due to interaction with SiO_2 cage. Polarization angular dependence indicates that PL has electric dipole character. Apart from the libration movements of O_2, the partial depolarization is caused by twofold orbital degeneracy of $a^1\Delta_g$ state. The cage-induced splitting of this degeneracy depends on cage size distribution and is calculated to be ≈ 0.1eV.

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PO-48

Luminescent Characteristics of Magnesium Aluminate Spinel of Different Stoichiometry

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Magnesium aluminate spinel (MAS) is a fascinating material with very high tolerance against radiation and absence of swelling even after heavy fast-neutron irradiation [1]. Therefore, $MgAl_2O_4$ crystals and transparent ceramics are considered as attractive candidates for diagnostics/optical windows in future fusion devices (ITER, DEMO, PROTO). MAS is a mixed double oxide $MgO \cdot nAl_2O_3$ and may be regarded as a face-centered cubic structure formed by oxygen ions. In stoichiometric MAS ($n = 1$, $MgAl_2O_4$) Mg^{2+} ions occupy every eighth tetrahedral (T) interstice and a half of octahedral (O) ones are filled by Al^{3+} in each unit cell. In a "normal" $MgAl_2O_4$, there is no cation disorder, while exchanging the cations between T and O sites results in the formation of antisite defects – $Mg|_{Al}$ or $Al|_{Mg}$. In nonstoichiometric MAS ($n > 1$, Al-rich), Al^{3+} replace Mg^{2+} with the creation of $Al|_{Mg}$, while some cation vacancies (mainly O-coordinated) additionally are formed for charge compensation [2].

The present study deals with a comparative study of the cathodoluminescence (CL) spectra in magnesium aluminate spinel samples with $n = 1$ and $n = 2.5$. CL spectra were measured at 6 K and 295 K under the same conditions (10 keV, 0.1 μA) for virgin and fast-neutron irradiated samples [3] and compared with the existing photoluminescence spectra (see also [4] and references therein. In order to analyze the origin of as-grown structural defects, the spectra and decay kinetics of phosphorescence as well as the thermally stimulated luminescence (TSL, integral signal or emission spectra within different TSL peaks) have been measured for single crystals with different stoichiometry after low-temperature 10-keV electron irradiation.

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PO-49

Single Step Preparation of Phosphorescent Coating on Aluminum

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Strontium aluminates are the most popular modern phosphorescent materials exhibiting long afterglow at room temperature as well as broad spectral distribution of luminescence in visible range. However, despite the great amount of research done, methods for synthesis of such materials remain relatively energy inefficient, environmentally unfriendly and are not optimized for majority of practical applications where phosphors are used as coatings.

For the first time the approach to produce phosphorescent strontium aluminates coatings on metal surfaces is demonstrated. The long afterglow luminescent coating containing $SrAl_2O_4:Eu^{2+}$, Dy^{3+} is prepared by the plasma electrolytic oxidation method on the surface of commercial and widely used aluminum alloy Al6082. During the electrical discharges in this process, the strontium aluminate is formed in a similar way to the solid-state reaction method. X-ray powder diffraction analysis confirms that monoclinic $SrAl_2O_4$ phase is present in the coating.

Some overview of phosphorescent PEO coating research will be provided as well as possible practical applications will be discussed.

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PO-50

Optical Investigation of the OH^- Groups in the Layers of $LiNbO_3$ Crystals Formed by Copper Ions Diffusion

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Lithium niobate *(*LiNbO3 *or* LN) is one of the well-developed active optical materials and finds wide application in electro-, acousto-, nonlinear and guided-wave optics. Some of these applications require single or double impurity doping, particularly, by hydrogen or copper ions. Actually, as it is well established, in LN crystals protons always appear in the form of $OH^–$ groups. These groups play a very important role in the thermal fixing of holograms, while their shape and peak position evidenced the chemical composition of LN and the presence of impurities [1]. Diffusion doping of LN by Cu ions is used for formation of memory elements or waveguides. According to the results of optical studies, it is proved that Cu^+ and Cu^{2+} incorporate into LN at the depths up to 800 μm at 600-800 °C and their distribution curves have got the Gaussian form. However, the spatial changes of the optical absorption of $OH^–$ groups in diffusion layers were not investigated yet. The aim of this work is the determination of the changes of position and shape of $OH^–$ groups absorption bands with the depth of the diffusion layer and the comparison of the obtained results with the spatial distributions of Cu ions. The bulk samples of LN were placed into CuO powder and annealed for 21 h in air at 800 K. The IR absorption spectra are investigated on the polished plate of LN (7(X)×15(Y)×16(Z) mm), using the special equipment allowed to record these spectra through 70 μm width diaphragm with the step of 20 μm. The spatial distributions of the absorption of OH^- groups were recorded in the directions perpendicular to the directions of Cu diffusion. As well as in [2], three absorption bands with maxima near 3448, 3478 and 3496 cm^{-1} are distinguished in the spectrum. The shapes and the positions of the bands are different for the different distances from the sample edges. The nature of the changes of OH^- group absorption in relation to the ones of Cu concentration in the diffusion layer is discussed.

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PO-51

Luminescence Properties and Decay Kinetics of Mn^{2+} and Eu^{3+} Ions in $MgGa_2O_4$ and $ZnGa_2O_4$ Ceramics

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$MgGa_2O_4$ and $ZnGa_2O_4$ spinel compounds are perspective materials for a different kind of displays and LEDs showing several principal advantages over commonly used sulfides [1]. Mn^{2+} ions are commonly used in efficient green phosphors [1, 2]. Moreover, co-doping these gallates with Mn^{2+} and Eu^{3+} ions provides an excellent opportunity to obtain radiation colors, from blue to red, depending on the concentrations of activators [2].

$MgGa_2O_4$ and $ZnGa_2O_4$ ceramics doped with 0.05 mol.% Mn^{2+} ions as well as co-doped with 0.05 mol.% Mn^{2+} and 0-8 mol.% Eu^{3+} ions have been successfully synthesized via a solid-state reaction method. The samples were characterized by X-ray diffraction, photoluminescence (PL) spectroscopy and PL decay measurements.

In the case of Mn^{2+} doped ceramics, an intense broad emission band at about 505 nm corresponding to Mn^{2+} centers has been observed under UV and blue light excitations. Excitation of Mn^{2+} and Eu^{3+} co-doped samples in UV charge transfer band ($O^{2-}\rightarrow Eu^{3+}$) or at 393 nm ($^7F_0 \rightarrow {}^5L_6$ transition in Eu^{3+} ions) yields addition bright orange-red emission.

It was found, that the Mn^{2+} lifetime is independent on Eu^{3+} ion concentration and remains almost constant at a value of ~ 7.4 and 5.1 ms for $MgGa_2O_4$ and $ZnGa_2O_4$, respectively. At the same time, the increasing of Eu^{3+} ions concentration in the spinel hosts results in a slight decrease of Eu^{3+} luminescence lifetimes. The decay constants as a function of excitation wavelength were also obtained. Possible mechanisms of energy transfer between the host lattice and the activator ions will be discussed.

Acknowledgements: the work was supported by the Ukrainian Ministry of Education and Science in frame of the Latvian-Ukrainian Joint Research Project (LV-UA/2016/1 in Latvia, and M/78-2017 in Ukraine) and the project DB/RIDER (no. 0117U004443).

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PO-52

Time Resolved Pulsed OSL Readout of Ceramic YAP:Mn Detectors

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Recently, application potential of Mn^{2+}-doped $YAlO_3$ (YAP) for thermoluminescent (TL) dosimetry of ionizing radiation has been successfully demonstrated (see [1] and references therein). On the other hand, the possibility of the pulsed optically stimulated luminescence (POSL) readout of this materials has been also implemented [2]. Until recently, the most of the research on YAP:Mn was carried out on Czochralski-grown single crystals. Only a while ago, it was shown that the solution combustion synthesis could be an appropriate method for obtaining of the Mn^{2+}-doped nanocrystalline YAP with high TL efficiency [3].

The present work reports the recent results of the time resolved pulsed OSL (TR-OSL) readout of the ceramic YAP:Mn detectors prepared from the nanocrystalline material synthesized by the solution combustion method [3]. For this purpose the compact POSL reader specially designed for YAP:Mn crystals [4] has been used. An intensity and shape of the TR-OSL signal from the YAP:Mn ceramic samples after X-ray (40 keV) irradiation is compared with that from the single crystalline detectors of similar nominal composition. It was observed that the shape of the TR-OSL signal from the ceramic samples changes essentially during the first 20-30 pulses of stimulation, thus demonstrating an important role of shallow electron traps that are more pronounced in the ceramics than in single crystals. The effect of preliminary heating of the detectors is also studied. The obtained results were compared with the TL response studied before for the ceramic detectors.

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PO-53

Radiation Impurity Defects in the Activated Potassium Sulphate Crystals

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Key words: ionic crystals, potassium sulphate, absorption spectrum, impurity ions, defect.

K_2SO_4 crystals, as well as potassium dihydrophosphate (KDP) is a crystal with the composite anionic complex. Due to the practical application of these crystals in the last decades specific features of characteristic and impurity electronic exaltations [1] are widely investigated. In the row the oxianionic crystals the conduction area is formed from excited states of cations and anions. Absorption spectra of the transitional metals of crystals of potassium sulphate activated by ions were for this purpose measured.

The crystal absorption spectrum K_2SO_4-Co^{2+} received at ambient temperature which is well coordinated with the result given in work [2]. The emergence of absorption bands in the crystals of potassium sulphate activated by Co^{2+}, Ni^{2+} and Mn^{2+} in the field of the matrix transparence according to [3] can be connected to the individual impurity centers. Exaltation of exemplars in these strips does not lead to emergence of photoluminescence. Measurement of photoconduction in a short-wave absorption band for K_2SO_4-Cu^{2+} crystal showed that it is not a charge transfer strip.

Similar results were received for K_2SO_4-Ni^{2+} и K_2SO_4-Mn^{2+} crystals at exaltation in short-wave absorption bands. The activated -Co^{2+}, K_2SO_4-Ni^{2+} and K_2SO_4-Mn^{2+} the absorption spectra are measured at ambient temperature are qualitatively similar.

Thus, the impurity ions of the transitional metals Me^{2+} (Co, Ni, Mn) are the centers of electron capture in K_2SO_4. These impurity ions influence emergence of padding cationic vacancies in a crystal.

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PO-54

Luminescence of K_2SO_4 Crystals Doped by Ions of Divalent Rare-earth Elements

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Optical and thermoactivation spectroscopy methods have experimentally investigated the spectral-luminescent properties of potassium sulfate crystals activated by europium ions. The nature of the emission band with a maximum at 3.1 eV and its corresponding excitation band with maxima at 3.8 eV and 4.4 eV is investigated. It was established experimentally that the thermal treatment of K_2SO_4-Eu $(NO_3)_3$ crystals does not lead to a redistribution of the intensities of the optical bands in the emission spectra and the excitation of photoluminescence.The most effective photoluminescence under the given conditions is excited in the long-wave band - with a maximum at 3.8 eV. To establish the nature of the optical bands, single crystals of potassium sulfate were grown when KNO_3 was added to the initial solution.

It has been experimentally established that in these crystals of potassium sulfate optical bands in the emission and photoluminescence excitation spectra are not observed. Crystals of K_2SO_4-KNO_3 in the range 200-800 nm do not have absorption bands.

Consequently, in the K_2SO_4-Eu $(NO_3)_3$ crystals, the observed photoluminescence is due to europium ions.

PO-55

Nanoporous Characterization of Modified Humidity-Sensitive MgO-Al_2O_3 Ceramics by Positron Annihilation Lifetime Spectroscopy Method

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The positron annihilation lifetime spectroscopy (PALS) is method for investigation of free volumes (nanopores) in materials [1]. In the case of ceramics, two channels of PALS should be considered – the positron trapping and o-Ps decaying. The aim of this work is study PALS characteristics of MgO-Al_2O_3 ceramics (sintered at T_s of 1100, 1200, 1300 and 1400 °C during 2 h) affected to water sorption treatment (Fig. 1).

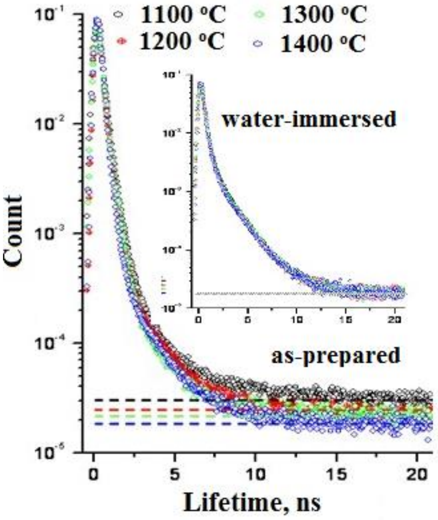

Fig.1 Peak-normalized PALS of MgO-Al_2O_3 ceramics sintered at 1100 °C, 1200 °C, 1300 °C and 1400 °C.

It is established that in all water-immersed samples, the intensity of third component I_3 significantly increases as compared with dried samples indicating a large content of absorbed water present in ceramics. The radius of free volumes where o-Ps are trapped in ceramics was calculated using the Tao-Eldrup model with character lifetimes τ_3 and τ_4. With increasing of ceramics sintering temperature T_s, the free volume radius R_3 increases from 3.09 to 3.31 Å and R_4 left nearly at the same level (~18 Å) in the samples taken after initial drying. In water-immersed samples, both nanopore radii R_3 and R_4 decrease with amount of adsorbed water. Thus, both types of inner nanopores in MgO-Al_2O_3 ceramics are practically identical in respect to efficiency of water sorption, but primary functionality of these ceramics is defined by smaller nanopores (defined by third PALS component) due to their prevailing content.

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PO-56

Structural Investigation of Crystallized Ge-Ga-Se Chalcogenide Glasses

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Ge-Ga-Se chalcogenide glasses are known as suitable materials for potential applications in IR photonics, etc. In the present research, we apply the X-ray diffraction (XRD), positron annihilation lifetime (PAL) spectroscopy, atomic force microscopy (AFM) and scanning electron microscopy (SEM) methods in order to perform structural investigation of $80GeSe_2$-$20Ga_2Se_3$ chalcogenide glasses thermally-activated at 380 °C for 25, 50 and 80 h.

It is shown that the structural changes caused by crystallization can be described by positron trapping modes. The observed changes in defect-related component speaks of structural fragmentation of larger free volume entities into smaller ones. In respect to XRD data, with increasing annealing time from 25 h to 50 and 80 h, the crystalline peaks at $2\theta \sim 28°$ are observed (Fig. 1). Peaks positions are in good agreement with $GeGa_4Se_8$ phase indexation. The size of nanocrystalline inclusions is near 9–10 nm. Crystallization of $GeSe_2$ phases in form of wires with length near 1-3 μm is a surface phenomenon (Fig. 2). The continued crystal evolution for longer durations of annealing is revealed by decrease in optical transmittance and long-wave shift of optical absorption edge of the studied glasses.

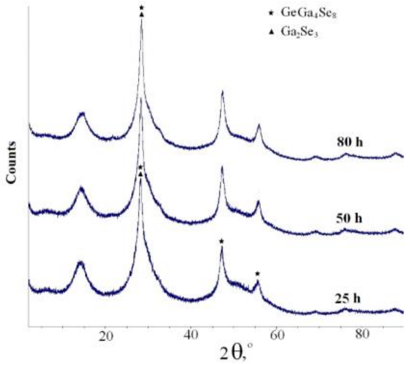

Fig. 1. XRD patterns of $80GeSe_2$-$20Ga_2Se_3$ glass annealed at 380 °C for 25, 50, 80 h

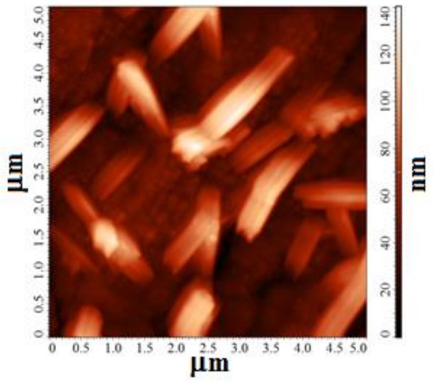

Fig. 2. AFM images of $80GeSe_2$-$20Ga_2Se_3$ glass annealed at 380 °C for 80 h

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PO-57

Wavefront Recovery from Intensity Measurements Using a Single Amplitude Modulating Mask

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It is known that detectors can only measure intensity while information about phase is lost. This is known as the phase problem and is faced in many areas of science including crystallography, astronomy, biology, optical communications etc. The information about the phase is crucial for determining the structure of the object under study and various methods have been proposed to solve the phase problem. Recently, an algorithm called *PhaseLift* [1] recovering the structure of the object very limited number of coded diffraction patterns was proposed. The algorithm works by finding a rank-one matrix and is based on low-rank Riemannian optimization methods [2].

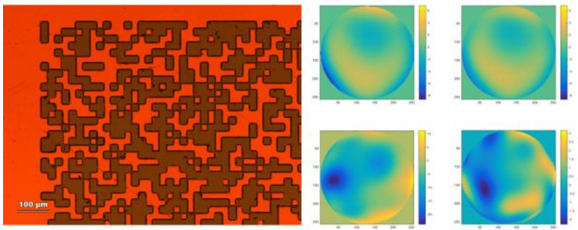

Fig.1 Left – the binary mask designed used the direct write lithography. Right – simulations of the wavefront reconstruction (upper row) and wavefront reconstruction from real measurements (lower row.)

In this study, simulations of wavefront reconstruction using a single binary mask were first carried out. Next, random structures in a photoresistive layer (photoresist AZ40-XT-11D) were created using the direct write lithography to distort a wavefront. A reference wawefront was calculated by propagating the angular spectrum of the wavefront just behind the wavefront modulator. The wavefront was modulated by a random amplitude modulating mask designed in a Cu layer. Simulations showed a nearly perfect reconstruction of the initial wavefront. Real measurements showed moderate correlation and noisy reconstruction probably due to the low number of modulating masks, detector noise and undercut of the mask. However, the noise could be easily filtered out by fitting the wavefront with Zernike polynomials.

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PO-58

Enhancement of Photosensitivity in Azo-epoxy Resists for Direct Holographic Recording

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Direct surface relief grating formation during holographic recording in azo-epoxy glasses is investigated. Azo-epoxy resist is promising material for direct holographic recording due to good photosensitivity and possibility to modify structure of molecule during synthesis – obtained polymer polymerization index easily can be changed by varying curing temperature of curing time. It allowed producing resist with low-weight molecular glasses properties. Resist was made for widely available laser with wavelength λ = 532 nm [1-3].

In this work 4-Aminoazobenze (AAB) and epoxy resin bisphenol A diglycidyl ether (BADGE) were used. For improving photosensitivity for wavelength λ = 532 nm Disperse Orange 3 (DO3) was added. Surface relief grating formation by direct holographic method was performed in obtained resists.

Surface relief grating post-recording self-enhancement process was investigated [4]. It allows increasing depth of surface relief grating after holographic recording, using physical method – uniform light illumination. It decreases time of holographic recording and consequently, required exposure for recording, making holographic recording more effective because grating formation is less affected by vibrations and noises.

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PO-59

Photoinduced Mass Transport in Amorphous Chalcogenide and Azobenzene Organic Materials

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The direct surface patterning of amorphous chalcogenide and low molecular organic glass films induced by polarization direction modulated optical field was studied. The influence of the amorphous film thickness, recording laser wavelength in the spectral range of (375 nm – 671 nm), grating period, recording light intensity and polarization state on the relief formation process in amorphous chalcogenides (As-S, As-S-Se, As-Se and Ge-Se systems) films was evaluated and compared with the measurements of azo-benzene containing low molecular organic glass films [1]. The best efficiency of surface relief grating (SRG) formation was observed with ($+45^0$, -45^0) and (RCP, LCP) polarized beam combinations, which involve primarily variation in linearly polarized state across the film - parallel and perpendicular regarding the grating vector. The relief grating profile on amorphous films was analyzed by means of atomic force microscope (AFM).

The phase relationship between the exciting light field and the resulting surface deformation was studied. It was observed that the peak of the SRG on chalcogenide films was formed at the position of p-polarization state in the polarization modulation pattern. It was shown that the efficiency and direction of mass displacement is determined by a value and sign of photoinduced birefringence in amorphous films. This fact is crucial to clarify the direction of the forces in SRG formation processes.

Holographic as well as the one beam methods for the grating recording [2] enable a fabrication of the gratings with a period from 100 nm up to 50 μm. A practical application of organic and inorganic optical recording photoresists for surface *direct* patterning will be discussed.

The mechanism of the direct recording of surface-relief on amorphous films based on the photoinduced softening of the matrix, formation of defects with enhanced polarizability, and their drift under the optical field gradient forces has been discussed.

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PO-60

Improvement of Diffraction Parameters in Surface Relief Holograms

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The holographic self enhancement (SE) for the holograms (HG) recorded under intensity modulated light illumination is well known and widely studied phenomenon for different kinds of structures. The object of presented work is studies for the similar behaviour on the surface relief holograms (SRHG) induced by the light electric field modulation. It should be noted that SRHG are strongly polarization sensitive, i.e., the recording, reading and enhancing depends on light beam polarization conditions.

In this work as base material ≈ 3μm thick azo-epoxy films were used. The kinetics for recording and SE under wavelength λ=532 nm influence at different involved light beam polarization states was tested. The influence of assisting light illumination was inspected as well. Fig.1 shows surface relief depth Δh for holograms recorded with constant (E ≈ 15 J/cm^2) light energy doses at p-p (1a) and ±45^O (2a) light beam polarization and then enhanced by one of recording beams at p polarization up to constant SE energy dose (E ≈ 1.1 kJ/cm^2). Wave-length λ of s polarized assisting light was 491 nm, intensity I=0.04W/cm^2.

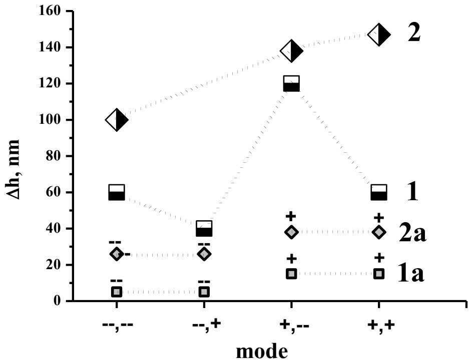

Fig.1 Surface relief depth Δh before and after SE for recorded with p-p (1a→1) and ±45^O (2a→2) polarized light beams. With marks -- or + is indicated the lack or presence of assisting light during corresponding process – first mark is related to recording conditions and second one – to enhancement respectively.

The motivation of presented work was to found the optimal recording and enhancement conditions for improving the diffraction parameters for primary two beams recording at low as possible light intensities end energy doses. That is necessary rule for achieving the real adequate size hologram recording.

PO-61

Search for Defects in $SrAl_2O_4$:Eu,Dy Material

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$SrAl_2O_4$:Eu,Dy, as well as other aluminates doped with europium, are very efficient long afterglow phosphors with wide range of possible applications – emergency signage, watch dials, luminous paints, in vivo imaging, etc.[1] The long lasting afterglow in $SrAl_2O_4$:Eu,Dy material is usually considered to be due to the thermal release of charge carriers from some kind of defects and the consequent recombination from the luminescence center Eu. We have conducted our research to investigate the mechanisms governing the long-lasting luminescence and the defects in the material that might take part in the processes. X-ray excited luminescence of $SrAl_2O_4$, $SrAl_2O_4$:Dy and $SrAl_2O_4$:Eu,Dy samples has been measured, including the measurements of afterglow at low temperatures within extended time scale. The study of afterglow kinetics reveals that electron tunneling from some trap to Eu^{3+} is involved in the creation of the excited state of Eu^{2+} [2]. In recent articles the tunneling of electron from trap levels to excited Eu luminescence center was discussed [2], and we conclude that under X-ray irradiation Eu^{2+} and Dy^{3+} serve as hole traps; electron tunneling is present in both $SrAl_2O_4$:Eu, Dy and $SrAl_2O_4$: Dy, and luminescence afterglow at 10 K arises from decay of excited Eu^{2+} and Dy^{3+} centers created via electron tunneling from host trap to Eu^{3+} and Dy^{4+} ions.

We also conducted spectral measurements of undoped material in order to understand the nature of traps in the material and if they are present in both doped and undoped material. We observed a clearly distinguishable luminescence of undoped $SrAl_2O_4$material under X-Ray excitation up to RT. The luminescence of undoped $SrAl_2O_4$ consists of two main parts – trace impurity metal, namely, Cr^{3+} luminescence, and intrinsic defects luminescence: F - centers and F_2 - centers. There is a strong possibility, that in the $SrAl_2O_4$ material these defects might be present as well and we propose that the presence of these defects is stimulating the Eu^{3+} ion incorporation.

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PO-62

Tailoring of Thermoelectric Properties of Bi_2Se_3 Thin Films by Adjustment of Dopant Concentration

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As the environmental impact of global climate change due to the combustion of fossil fuel is becoming increasingly alarming, one of the possible ways to improve the sustainability of the world's electricity base is conversion of the enormous amount of waste heat directly to electricity, using thermoelectric energy conversion devices. Bismuth chalcogenides – a group of materials of the general formula $Bi_2(Te,Se)_3$ - are very intensively studied as the best TE materials operating near room temperatures (200-400K), which are extremely important for Peltier cooling and domestic waste heat-to-power conversion applications. However, the state-of-the-art TE efficiency of these materials is not high enough for commercial applications.

As it is well-known, the efficiency of TE materials is characterized by dimensionless parameter, which is denoted ZT (figure of merit) and is a combination of material's Seebeck coefficient, electrical and thermal conductivities. One of the ways to enhance ZT of bismuth chalcogenides is to combine their downsizing with specific doping. Recently, doping of bismuth chalcogenides with Cu and Sn in combination with co-doping compensating their natural n-type defects was proposed as a perspective path for reduction of their thermal conductivity and introduction of a resonant impurity levels in their structure, which may result in significant enhancement of their ZT [1].

In this work, the bismuth selenide thin films are fabricated by developed in the Institute of Chemical Physics catalyst-free deposition technique [2], allowing natural compensation of n-type defects down to the "low-doped" Bi_2Se_3 crystal level, optimal for the TE applications. TE performance of these films is tailored by introduction of different concentrations of specific dopants during the deposition process. Doped bismuth chalcogenide thin films show enhanced TE performance in comparison with non-doped and bulk material. Dependence of TE prerformance on dopant concentration is discussed.

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PO-63

Thermoelectrical Properties of NBT Ceramics

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Lead-based ceramic materials as PZT, commonly used so far, due to the content of toxic lead, should be replaced by lead-free materials. One of the materials that can replace lead-based materials is discovered by Smolensky et al. $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) [1]. However, the NBT piezoelectric properties are not as good as piezoelectric properties of PZT [2,3]. In order to improve the NBT properties, there are many NBT-based materials investigated (e.g. NBT-$BaTiO_3$ [4,5], NBT–ST [6]). Another way to improve the NBT properties is to obtain this material using different sintering conditions [7,8].

The investigated lead-free $Na_{0.5}Bi_{0.5}TiO_3$ ceramics were produced by conventional solid – state reaction method and during the hot-pressing route. The structural measurements, Seebeck coefficient, ac (σ_{ac}) and dc (σ_{dc}) conductivities were studies to investigated the influence of sintering conditions of these properties. The X-ray measurements showed that all investigated samples have a perovskite structure. Obtained spectra of these samples are similar to each other, however, some differences were observed. The conductivity measurements obtained for all examined samples show that the numbers of sintering or hot-pressing route affect the conductivity values. Also the Seebeck coefficient shows, that the influence of sintering conditions on properties of investigated samples is noticeable.

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PO-64

Effects of CuO Doping on Structure, Microstructure and Dielectric Properties of $BaTiO_3$-$PbTiO_3$ Solid Solution

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$BaTiO_3$ is one of the most known ferroelectric oxides due to its exceptional electrical properties and find applications among others as ultrasonic transducers, thin-film memories multilayer ceramic capacitors. The electrical properties of pure barium titanate may be altered by doping (there are multiple incorporation mechanisms for dopants in the perovskite structure). The electrical characteristic of $BaTiO_3$ also depend on the site of substitution. The introduced cation may behave like donor if occupies Ba^{2+} site or like acceptor if it takes a titanium Ti^{4+} ion site. In addition this type of doping is also a reason of the formation of multiple defects.

$BaTiO_3$, $(1-x)BaTiO_3$-$xPbTiO_3$ and $(1-x)BaTiO_3$-$xPbTiO_3$+(y)wt%CuO samples were prepared by solid state reaction method. High purity of raw materials were used. Structural properties of the sintered pellets by X-ray diffractometer X'Pert PRO (PANalytical) were studied. The Rietveld refinement was carried out using Fullproof software. A single phase of perovskite structure with tetragonal phase was identified at room temperature. The surface morphology of the obtained specimens was characterized by a scanning electron microscopy (Hitachi S4700). The results of the chemical composition was carried out with the use of EDS measurements. The investigations shown that the synthesized ceramic materials, characterized by the high density, homogeneity of microstructure and low porosity. Dielectric measurements were carried out using an Alpha-AN High Performance Frequency Analyzer combined with cryogenic temperature control system (Quatro Cryosystem) in the temperature range from 140 K to 600 K. The frequencies varied from 0.1 Hz to 10 MHz at applied voltage 1 V. Nitrogen gas was used as a heating and cooling agent.

PO-65

The Effect of Sr Modification on Mechanical Properties of $Na_{0.5}Bi_{0.5}TiO_3$ Ceramics

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In lead-free ceramic systems, $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) can potentially replace lead-based materials because of the presence of stereo-chemically active lone-pair electrons of Bi [1, 2]. $N_{0.5}Bi_{0.5}TiO_3$-$SrTiO_3$ (NBT-ST) is a solid solution system composed of ferroelectric NBT and non-ferroelectric ST, both of them are of perovskite structure. For device design and theoretical analysis, it is necessary to know a complete set of dielectric, piezoelectric and mechanical properties. However, in the literature, only dielectric and piezoelectric properties are reported, mechanical properties have not been measured up to date [3].

Lead-free (1-x)NBT-xST (x=0-0.1) ceramics were synthesized by a conventional mixed-oxide route. The ceramics possess a single-phase perovskite structure with rhombohedral symmetry. The microstructure study showed a dense structure in good agreement with the measurements by the Archimedes method. The relative densities were above 96 % of theoretical values. Based on the measurements of the velocities of the longitudinal and transverse ultrasonic waves propagation the Young's modulus (E), the shear modulus (G), the bulk modulus (K) and the Poisson ratio (ν) were determined. It was found that the relations G/E~3/8 (0.379) and K/G~5/3 (1.57) valid for isotropic homogeneous ceramics material are fulfilled. The performed measurements indicated that the addition of Sr^{2+} ions to NBT rather affects slightly the mechanical properties.

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PO-66

Characterzation of $SrTiO_3$ - $SrHfO_3$ Solid Solution by Dielectric Spectroscopy

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The search for new dielectric materials, exhibiting both, temperature and frequency stable, as well as sufficiently low dielectric loss, are continues to arouse considerable interest because of their numerous applications. The results of the research on the influence of the substitution, in cationic sublattice (strontium titanate), Hf^{+4} ions on the electric properties in the $SrTiO_3$ - $SrHfO_3$ (STH) solid solution are presented.

The $SrTiO_3$ - $SrHfO_3$ ceramics have been obtained from oxides by means of conventional high-temperature solid state synthesis method. The structure and morphology of the investigated samples were characterized by an X-ray diffraction (XRD) and scanning electron microscopy (SEM). Characterization of electrical properties of STH samples within the temperature range 153 K ÷ 573 K were performed by means of dielectric spectroscopy method within the frequencies from 0.01Hz to 10MHz. Analysis of temperature and frequency dependences of real and imaginary parts of dielectric permittivity, electric modulus as well as impedance, provided the new details about specific features of physical properties of ceramic samples.

PO-67

Preparation and Dielectric Properties of $(Na_{0.5}K_{0.5})NbO_3$ Ceramics with ZnO and CdO Addition

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ABO_3-type compounds with perovskite structure are one of the most interesting group of materials. Among them niobates are of great interest from the point of view of fundamental research as well as of their possible applications. Especially the potassium sodium niobate ceramics with high Curie temperature, good dielectric properties and high piezoelectric coefficients are considered as one of the most perspective candidate materials to replace highly effective lead-based materials. $(Na_{0.5}K_{0.5})NbO_3$ (NKN) is a solid solution of ferroelectric $KNbO_3$ (KN) and antiferroelectric $NaNbO_3$ (NN). Both of these compounds show orthorhombic symmetry at room temperature.

At present the main problem concerning NKN is sintering process. It is difficult to obtain samples with a high density by using a conventional methods, among others due to the high volatility of alkaline elements at high temperatures. In this case to produce well sintered, dense ceramic with one phase there was added 1%wtZnO or 1%wtCdO as sintering aid.

The sintering conditions, phase structure, and electrical properties of the pure $NaNbO_3$, $(Na_{0.5}K_{0.5})NbO_3$ and ZnO, CdO doped $(Na_{0.5}K_{0.5})NbO_3$ ceramics were investigated and discussed. All samples were prepared by solid state reaction method. The phase structure was investigated with an X-ray diffraction analysis. Densities of the samples were measured by Archimedes method. The investigations of the microstructure of polycrystalline ceramic specimens were performed on fractured surfaces by using the Hitachi S4700 Scanning electron microscope. The X-ray microanalysis Energy-Dispersive X-ray Spectroscopy was applied to investigate the homogeneity of the composition and the Electron Probe Microbeam. Dielectric measurements were carried out using an Alpha-AN High Performance Frequency Analyzer.

PO-68

Effect of Cu Doping on the Electrical Properties of $Ba_{0.95}Pb_{0.05}TiO_3$ Ceramics by Means of Impedance Spectroscopy

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The $Ba_{0.95}Pb_{0.05}TiO_3$+Xwt.%CuO (X=0, 0.05, 0.1, 1, 3) ceramics were prepared by a solid phase reaction. The structural and morphology studies were carried out by means of an X-ray diffraction technique and scanning electron microscopy, respectively. The thermal parameters of the transition were also estimated and discussed. The electrical properties of the materials were determined by electrochemical impedance spectroscopy (EIS). Sintered bodies equipped with commercial silver paste electrodes were examined in synthetic air atmosphere using a frequency analyzer (Solartron FRA 1260) coupled with Dielectric Interface (model 1296) in temperature range 473-773K. Frequency range was 0.1 Hz-32 MHz, the amplitude of sinusoidal voltage signal was 20 mV. The obtained Nyquists spectra were analyzed by fitting equivalent circuits parameters using dedicated Zview software (version 2.2, Scribner Associates, Inc.). For all specimens gradual modification of spectra shape were observed with the increase of temperature. At 473K spectra consisted of semicircle in high frequencies and arc in low frequencies, whereas at 773K three semicircles were visible. At lower temperatures the electrodes are blocking for oxygen. Thus processes taking place in grain interiors (bulk) and at grain boundaries of polycrystalline ceramic mainly affect the shape of spectra. At higher temperatures electrodes turn into reversible. Therefore oxygen ionization processes on three point boundary (gas-metal-ceramic) are exhibited in the low frequency part of the spectra as additional semicircle. The specific conductivities were established using values of resistance obtained by spectra analysis taking into account the specimens geometry. Additionally basing on Arrhenius plots, the linear regression analysis was performed and the energy of activation values were calculated. The direct comparison of specific resistance and energy of activation values for all specimens, enabled the determination of CuO doping impact on electrical conduction mechanism in (0.95BT-0.05Pb)TiO_3 ceramics.

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PO-69

Thermal Expansion and Polarization of (1-x)$PbNi_{1/3}Nb_{2/3}O_3$-x$PbTiO_3$ Solid Solutions

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The prospects of the PNN-PT solid solutions – (1-x)$Pb(Ni_{1/3}Nb_{2/3})O_3$-x$PbTiO_3$ - for applications are associated with high dielectric permittivity, large piezoelectric and electrostriction coefficients. The PNN belongs to multiferroic compounds of relaxor behaviour with $T_m \approx 153$ K and $T_N \approx 5$ K, respectively. Well-studied typical ferroelec-tric lead titanate undergoes cubic-to-tetra-gonal phase transition at $T_c \approx 750$ K. The T-x phase diagram of the PNN-PT system demonstrates a morphotropic region existing around x ~ 0.35 where several phases may coexist: the cubic, pseudo-cubic, tetragonal, and rhombohedral [1].

The present investigation describes the detailed studies of thermal expansion in the series of the (1-x)PNN-xPT solid solutions with x= 0 - 0.8 performed in the temperature range from 100 to 780 K. The anomalous and lattice contributions of deformation and the coefficient of thermal expansion are analysed and used to estimate the Burns temperature and the mean square polarization P_d (Figure 1). The obtained results are discussed within thermodynamic theory [2], and coefficients 2-4-6 of Landau potential for solid solutions are determined.

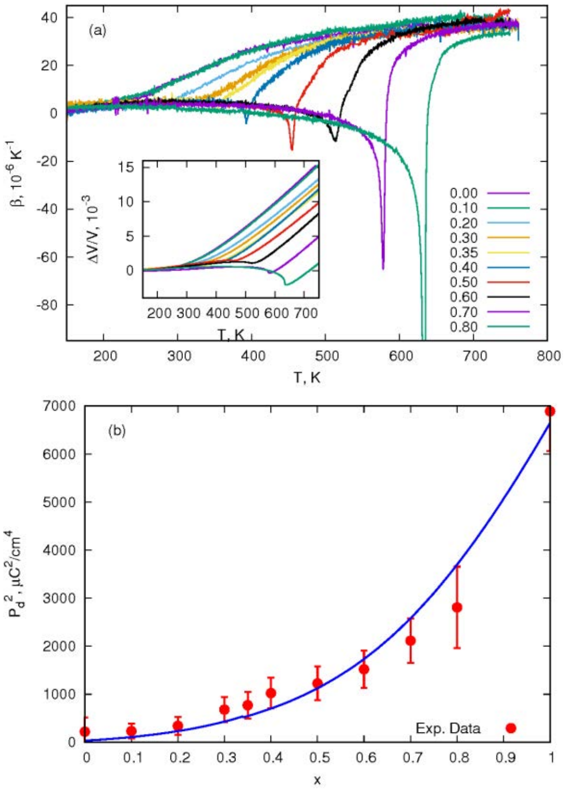

Fig.1. Thermal expansion (a) and polarization (b) of solid solutions (1-x)$PbNi_{1/3}Nb_{2/3}O_3$-x$PbTiO_3$

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PO-70

Dielectric Properties and ac Conductivities of $Bi_{1-x}Sm_xFeO_3$ Ceramics

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The research of the structure, frequency and temperature dependences dielectric properties and ac conductivities of $Bi_{1-x}Sm_xFeO_3$ (x = 0, 0.05, 0.1, 0.15, 0.20) ceramics are presented. BSFO ceramics were obtained by cold pressing of nanopowders thermally treated at 600°C. It is shown that BSFO-5 as well as BFO crystallizes in rhombohedral structure with R3c space group. XRD analysis of the composition BSFO-10 indicates the presence of a new orthorhombic (space group: Pbam) phase. With 15% bismuth's substitution, the crystal structure is completely transformed from rhombohedral to orthorhombic phase.

The measurements dielectric constant (ε'), loss tangent (tgδ) and ac conductivity (σ_{ac}) were carried out in the frequency range 1 kHz – 10 MHz in the temperature range 25 – 600 °C. Both components of ε undergo strong frequency dispersion. The intense temperature growth of the real part ε' begins above 200 °C, reaches its a local maximum at ~ 230 °C, and has a frequency-dependent character inherent to relaxors (Fig. 1). Its maximum value ε'(T) reaches at ~ 300 °C. Figure 2 shows the different conductivity character in different temperature and frequency ranges. At low frequencies and temperatures above 300 °C the conductivity of all BSFO compositions gradually increases up to 600 °C. Conductivity is higher for samples with a high samarium concentration. As can be seen from Fig. 2(b), the dependence $\sigma_{ac}(T)$ for 10 MHz reaches to saturation and passes through a maximum. Moreover, the conductivity maximum temperature is shifted to lower temperatures area with an increase in both the frequency and the percentage content of samarium. The form of $\sigma_{ac}(\omega)$ curves for BSFO at different temperatures indicates its thermoactivation character. The low-frequency conductivity is identified with the dc conductivity (σ_{dc}). At frequencies > 100 kHz conductivity behavior can be interpreted in frame of the model of correlated barrier hopping (CBH) of charge carriers.

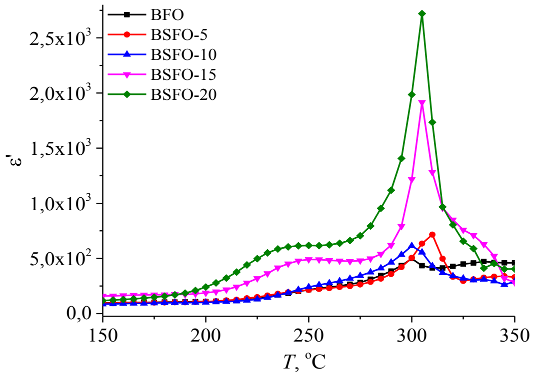

Fig.1. Thermal dependence of ε′(T) at 1kHz

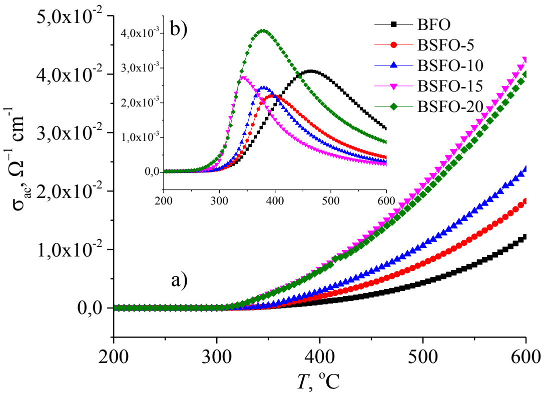

Fig.2. Thermal dependence of σ_{ac}(T) at 1kHz (a) and 10 MHz (b)

PO-71

Evolution of Domain Structure of $LiNbO_3$:ZnO Crystals During High Temperature Annealing

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$LiNbO_3$:ZnO crystals have been extensively studied due to their resistance to optical damage. Anomalous behavior of σ(T) dependences in $LiNbO_3$:ZnO crystals doped in the concentration range (~ 5.4 < $C_m \leq 6.8$ mol % in the melt have been previously reported. Jump-like increase in σ is observed at the temperature $T^{*}\approx800\pm10$K. The value of piezoelectric coefficient d_{333} of originally polydomain $LiNbO_3$:ZnO crystal increases to ~$16.2\bullet10^{-12}$ C/N. This value exceeds the maximum values in $LiNbO_3$ crystals artificially brought to single-domain state. The value of piezoelectric coefficient d_{333} jump linearly increases with the increase in conduction jump Δσ near the temperature T* ≈ 800 K. This paper compares conduction of $LiNbO_3$:ZnO and congruent $LiNbO_3$ crystals and studies the evolution of the domain structure of $LiNbO_3$:ZnO crystals caused by the conduction jump in the temperature range ~ 800K. Increase in the unipolarity range of $LiNbO_3$:ZnO crystals is accompanied by vanishing of the domain structure. Such structure reveals in $LiNbO_3$:ZnO crystals as a result of chemical etching. After annealing by short circuit, we have observed drastic increase in unipolarity degree. The value of piezoelectric coefficient d_{333} has also increased. Etching figures were only separate hexagonal microdomains ~ 1-3 μm in diameter. At the same time, the temperature behavior of conductivity and unipolarity degree is usual for nominally pure congruent $LiNbO_3$ crystals at T < ~ 900 K annealed by short circuit. Existence of anomalies of σ(T) dependences in $LiNbO_3$:ZnO crystals at quite certain temperature (~800±10K) confirms that the evolution of the domain structure starts by thermal decom-position of charged clusters that stabilize domain walls. This leads to the jump-like injection of extra charge carriers. Anomalous increase in conductivity in $LiNbO_3$ crystals at T* ≈ 800 K leads to the following: at T<800K, the conductivities of $LiNbO_3$:ZnO and congruent $LiNbO_3$ are comparable, at T>800K, the conductivity of crystal $LiNbO_3$:ZnO is one order of magnitude higher than that of congruent $LiNbO_3$. This is apparently the explanation of the changes in domain behavior of $LiNbO_3$:ZnO and congruent $LiNbO_3$ at high temperatures.

PO-72

Studies of Hydrogen Ion Bonds and Their Influence on Formation Structure of $LiNbO_3$:Mg and $LiNbO_3$:Zn Crystals

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Any $LiNbO_3$ single crystals grown in the air always contain hydrogen (H^+) in its structure. The behavior of OH^- groups in a crystal depends on the concentration and the type of a "nonphotorefractive" cation, which weakens the effect of the optical damage. Since the concentration of OH groups in the crystal is low, specific features of the localization of OH^- groups in a crystal and the associated changes in the structure can be investigated most easily by IR absorption spectra.

In the present paper on the IR absorption spectra for $LiNbO_{3congr}$, we investigated the effect on the valence vibration of OH groups of the dopants Mg^{2+} over a range of concentrations (0.19–5.91 mol % MgO) and Zn^{2+} over a range of concentrations (0.04 - 4.68 mol % ZnO). Note that the range of Mg^{2+} dopant concentrations studied includes two concentration thresholds, at ≈3.0 and 5.5 mol % MgO, whereas the range of Zn^{2+} concentration includes one threshold, at ≈2.0 mol % ZnO. It was found that the absorption bands in the IR spectra of $LiNbO_{3congr}$, $LiNbO_3$:Mg(0.19–5.91 mol % MgO) and $LiNbO_3$: Zn (0.04 - 4.68 mol % ZnO), where $Nb_{Li,}$ defects are located in the region of the stretching vibrations of the OH^-groups, are split into three components. This indicates various positions for the OH^- groups and various values for the quasielastic constant of the hydrogen bonds with the oxygen atom in the vacant octahedra and in the octahedra occupied by basic (Li^+, Nb^{5+}) and doping Mg^{2+} and Zn^{2+} cations. For the stoichiometric $LiNbO_3$ crystal, in the absence of Nb_{Li} defects, only single-mode behaviour is observed, since there is only one position of the hydroxyl group in the structure, which is characterized by a single quasi-elastic constant of the O–H bond, with its value being smaller than the values of the quasi-elastic constants of O–H bonds in nonstoichiometric crystals. The present results provide a conclusive evidence that there are concentration thresholds in the $LiNbO_3$:Mg crystals in the composition range of 3.02–5.9 mol % MgO and in the $LiNbO_3$:Zn crystals at ≈2.0 mol % ZnO.

PO-73

Photoelectric Fields in Doped Lithium Niobate Crystals

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Photoinduced light scattering (PILS) in nominally pure stoichiometric and congruent lithium niobate single crystals ($LiNbO_3$), the ones doped with B^{3+} (0.08 wt.% in the reacted mixture), and Cu^{2+}, Zn^{2+}, Mg^{2+}, Gd^{3+}, Y^{3+}, Er^{3+} cations was studied. All crystals have a relatively low effect of photorefraction and are promising materials for frequency conversion, electro-optical modulators and shutters.

The following laser lines were used in PILS experiment: 476.5 nm (P = 216 mW), 488.0 nm (P = 98 mW), 514.5 nm (P = 282 mW) of Spectra Physics (2018-RM) laser and 532.0 nm (P = 160 mW) of Nd:YAG MLL-100 laser. The diameter of the laser beam was 1.8 mm. In all cases, the geometry of the experiment was such as to register the PILS of *ee* type, i.e. incident and scattered radiation have the same polarization, and the vector *E* was oriented parallelly to the polar axis (Z axis). According to the characteristics of PILS, a quantitative estimate of the photovoltaic and diffusion field values was made using the approach described in [1].

It was found that the E_{pv} and E_d for some crystals have a maximum at a wavelength of 514.5 nm. All the crystals studied are characterized by a maximum of the integral intensity of the speckle pattern PILS indicatrix at a wavelength of 514.5 nm. However, for the $LiNbO_3$:Y (0.46 wt. %) crystal, which is characterized by anomalously rapid opening of the speckle structure of the PILS indicatrix (within 1 s), there is no maximum in the E_{pv} curve. At the same time, a maximum in the E_d at a wavelength of 514.5 nm was observed for $LiNbO_3$: Y crystal.

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PO-74

Optical Properties and Structure Particularities of $LiNbO_3$ Crystals Grown from Boron-Doped Melt

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Generally, doping means introducing some dopant into the crystal structure in a significant amount in order to change the physical properties of the material. Despite the fact that boron can be introduced in the charge at high concentrations (up to 2.0 mol%), it doesn't introduce to the structure of the $LiNbO_3$ crystal (the concentration of the boron in the crystal ~10^{-4} wt. %). Oxide compounds of boron, as strong complexing agents, have a significant influence on the structure and physical characteristics of the melt, and, consequently, on the structure of the grown crystal. The melting point of $LiNbO_3$:B crystals, grown from a boron-doped melt (1264 °C), increases compared to a nominally pure lithium niobate single crystal of a congruent composition (1257 °C). In the Raman spectra of $LiNbO_3$:B crystals significant changes were observed. These changes indicate both the ordering of cations and vacancies, alloying them along the polar axis of the crystal, and the "distortion" of the oxygen octahedra of the structure compared to the crystal of the congruent composition. The boron impurity, structuring the melt in a certain way, reduces the amount of Nb_{Li} defects and is likely to reduce the content of uncontrolled impurities. Thus, boron impurity reduces the photorefractive effect in a single crystal and increases its structural and optical uniformity.

Thus, for the first time, we have carried out an approach for obtaining single crystals of $LiNbO_3$ with given properties. In this case, the melt is ordered by the chemically active element in a certain way, but the alloying impurity doesn't enter the structure of the crystal. Using melt structuring, this approach allows us to receive nominally pure $LiNbO_3$ crystals having properties similar to doped crystals. In this case, boron-doped crystals approach the crystal of stoichiometric composition by ordering the structural units of the cation sublattice and defects Nb_{Li}. At the same time, the crystals $LiNbO_3$:B obtained possess significantly smaller photorefractive effect and noticeably greater structural and optical uniformity unlike stoichiometric crystals.

PO-75

Research of the Model of Lithium Niobate Cluster

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The creation of modern technologies for single-crystal materials and the study of the fine features of their structure, which significantly affect the quality of physical characteristics, require the addition of a physical experiment by virtual – computer modeling of micro- and nanostructures and their evolution with changing crystal composition.

Crystallization under conditions far from thermodynamic equilibrium in $LiNbO_3$ crystals, as well as changing the composition of the cation sublattice (by changing the Li/Nb ratio or doping) can generate domain structures of micron and submicron sizes, which determines the physical characteristics of materials based on the $LiNbO_3$ single crystal. In this case, a variety of dipole oxygen-octahedral clusters form in the crystal, direct experimental study of the structure of which presents considerable difficulties.

In calculations, we used oxygen octahedra instead of elementary cells, which allowed us to avoid the torn octahedra at the edges of the cluster. A function was obtained that describes the dependence of the number of octahedra (positions Li, Nb or vacancies) on the number of oxygen layers in the lithium niobate cluster. It is shown that the function has a minimum, which makes it possible to determine the most energetically favourable cluster size.

The performed calculations revealed the existence of a cluster of a certain size, which has a minimum of energy, and within which a structure tending to the structure of a congruent lithium niobate crystal is formed. With a congruent Li/Nb ratio, there is a minimum of energy, which proves the energy optimality of a congruent crystal. In addition, an optimal relationship between cluster energy, its size and the Li/Nb ratio was found.

It can also be seen from the calculations that a cluster of stoichiometric composition cannot exist, since it does not make it possible to preserve electroneutrality. Calculation of a cluster containing approximately 3500 ions leads to a maximum Li/Nb ratio, which is also the least energetically favourable. Further increase in the size of the cluster reveals a sharp decrease in its energy. The most energetically favourable are clusters of the order of 7000 ions.

PO-76

Grain Growth in $Na_{0.5}Bi_{0.5}TiO_3$-based Solid Solutions

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Demand for Na0.5Bi0.5TiO3-based solid solutions is increasing due to the fact that most ferroelectric solid solutions such as Pb(Zr1-xTix)O3 contain large amounts of lead, these solutions are toxic and can cause lead poisoning and environmental pollution [1]. Microstructure and properties of lead-containing solid solutions can be improved by using a variety of dopants in different concentrations and by varying parameters of the sintering stage. Sintering of ferroelectric solid solutions can cause rapid grain growth and expansion of grain size distribution which leads to abnormal grain growth. This abnormal grain growth reduces many Na0.5Bi0.5TiO3 properties such as hardness and reproductivity of microstructure.

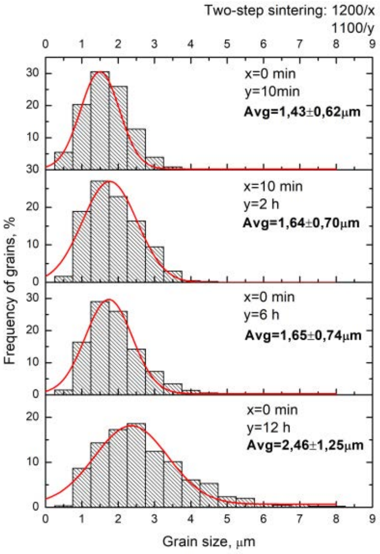

Fig.1 Grain growth distribution of different sintering times in two-step sintering

Microstructures of A-site doped Yb, Ce and Er-doped NBT solid solutions were studied. Small amounts of Yb and Ce increase average grain size remarkably, while Bi over-stoichiometry suppresses grain growth and facilitates unimodal grain size distribution, which can be explained by presence of liquid phase in Bi-overstoichiometry.

In addition to different variations in dopant types and concentrations, using such sintering techniques as hot-pressing, two-step sintering (Fig.1) and conventional sintering leads to microstructural divergency. Different sintering techniques such as Chen-Wang approach have shown to successfully suppress abnormal grain growth, thus inducing unimodal grain growth with maximum possible densification level.

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PO-77

Effects of Strong Electric Fields on Polarization and Structural Properties Changes of 3d-ion Doped PLZT 8/65/35 Ceramics

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Lanthanum-doped lead zirconium titanate ferroelectric compounds Pb1-yLayZrxTi1−xO3 (PLZT) are very interesting because of their high optical transparency important in various optical applications such as light shutters, electro-optical modulators, color filters, memories and imaging storage devices. Polarization in such ferroelectric materials can be characterized by dielectric permeability (ε) in weak electric fields, where E ≤3 V/cm, or by polarization hysteresis loops P(E) in strong electric fields, where the E range is 1-30 and more kV/cm.

In this report, a series of PLZT (8/65/35) ceramics with different 3 d ion concentration have been synthesized to figure out the effects of strong electric fields on polarization and observed changes of their structural properties [1]. All PLZT (8/65/35) ceramic samples were prepared by two-stage hot pressing from chemically co-precipitated raw materials synthesized from a mixture of main oxides with the necessary amount of 3d ion dopants (0.01; 0.1; 0.3; 1.0 and 3.0 wt.%)

We have performed a detailed analysis of the temperature dependencies of P(E) studied in temperature range from -60 to 150 ° C by changing: 1) E-amplitude, 2) E-frequency (Ef) (0.02 sec (50 Hz), 15 s, 1, 4, 16 min), 3) 3d (Cr, Mn, Fe, Co, Ni, Cu) dopant concentrations: 0.01; 0.1; 0.3; 1.0 and 3.0 wt.%. Depending on the type and concentration of the 3d elements, as well as on the temperature, significant and characteristic changes in the P (E) form were established. It is also established that there is the significant influence of the hot-pressing parameters on P (E) behavior. The influence of the dopant concentration on P (E) aging was also found, namely, we have observed the significant decrease of aging time in heavily doped PLZT samples. Finally, the multifaceted and complex effect of 3d- impurities and their specific roles on the observed P(E) dependences are analyzed in discussed in details.

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PO-78

Heat Capacity of Multiferroics $Bi_{1-x}Pr_xFeO_3$

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Heat capacity of multiferroics $Bi_{1-x}Pr_xFeO_3$ ($0 \leq x \leq 0.20$) was studied over a wide range of temperatures (130–800 K). Powders of $Bi_{1-x}Pr_xFeO_3$ were obtained by solid phase reactions from high purity grade oxides. The mixture was ground in ball mill mixed with ethanol during 24h and calcinated 2h at 1150 K. Ceramics were produced by conventional ceramic technology at 1200–1250 K. The synthesis and sintering phase constitution were examined by X-ray diffraction using a DRON-3 diffractometer with FeK_α and $CuK\alpha$ radiations. The heat capacity was measured using a NETZSCH DSC 204 F1Phoenix differential scanning calorimeter.

The X-ray phase analysis show that the pure solutions was formed at the Pr concentration $x \geq 0.12$; at lower x, the samples contained low concentrations of the $Bi_{25}FeO_{40}$ and $Bi_2Fe_4O_9$ compounds. Diffraction reflections reveal the several concentration ranges with different phase compositions. In the range $0 \leq x < 0.10$, the rhombohedral R3c phase inherent in $BiFeO_3$ exists. At $0.10 < x \leq 0.20$, three phases coexisted: the rhombohedral R3c and two orthorhombic P_1-type $PbZrO_3$ and P_2-type $GdFeO_3$ (the former phase was dominant). In the range $0.20 < x \leq 0.30$, phase R3c disappeared, and two phases P_1 and P_2 coexisted.

The results show that an insignificant substitution of praseodymium for bismuth markedly shifted the antiferromagnetic phase transition point to higher temperatures. The anomalies observed in the temperature dependences of the heat capacity for the compositions with x = 0.10, 0.15, and 0.20 compare with a structural data show the structural phase transitions. An additional contribution to the heat capacity in the temperature range 240–800 K appears in doped bismuth ferrite with rare-earth element Pr, and can be interpreted as the Schottky anomaly for three-level states. In the case of doping with rare-earth elements, a three-level system can form due to a distortion of the lattice parameters due to the polar displacements of bismuth and iron ions from the initial positions and a change in the bond angle between oxygen octahedra FeO_6. On the basis of the results of heat capacity, a phase diagram $T_N(x)$ for the system $Bi_{1-x}Pr_xFeO_3$ was formed.

PO-79

Oxygen Isotope Exchange with oxides $La_{1-x}Sr_xCoO_{3-\delta}$

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Oxygen surface exchange kinetics with oxides $La_{1-x}Sr_xCoO_{3-\delta}$ (x = 0, 0.3, 0.4, 0.6) has been studied by the isotope exchange method with gas phase equilibration using a static circulation experimental rig at oxygen pressure 0.67 kPa and temperatures 600-850°C.

The oxygen interphase exchange rate (r_H) increases with strontium concentration (x) in oxides $La_{1-x}Sr_xCoO_{3-\delta}$. In order to reveal the reason of r_H behavior with x oxygen dissociative adsorption rate (r_a) and incorporation rate (r_i) have been calculated in the framework of the two-step model. The oxygen incorporation rate increases significantly with x, since the concentration of oxygen vacancies increases. The oxygen dissociative adsorption rate has a less pronounced dependence on x, which is associated with two factors: doping strontium increases the volume of adsorptive layer, but blocks the adsorption centers due to segregation on the surface.

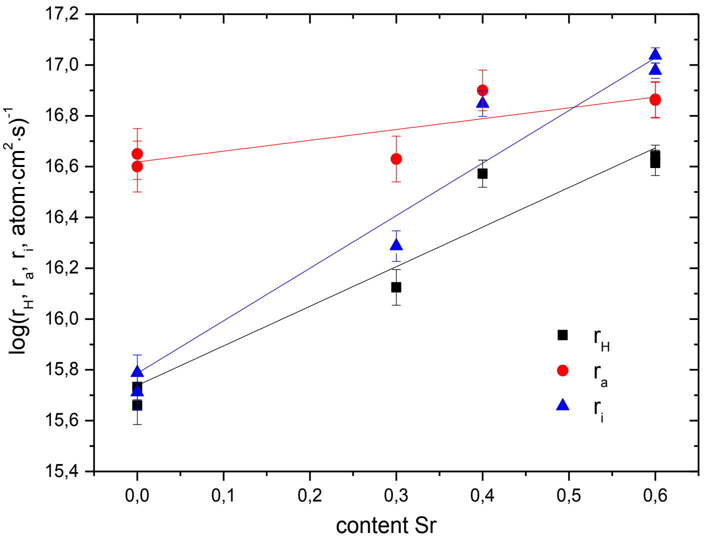

Fig. 1 Dependences of the oxygen interphase exchange rate (r_H), oxygen dissociative adsorption (r_a), and incorporation (r_i) rates on the content Sr in $La_{1-x}Sr_xCoO_{3-\delta}$ at T=700°C, P_{O_2}=0.67 kPa.

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PO-80

Electromechanical Properties of Some Relaxor-PT Solid Solutions

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Disordered perovskite oxides which exhibit relaxor properties are known for their excellent dielectric and piezoelectric properties. So far some of the relaxor ferroelectrics mixed with a canonical ferroelectric lead titanate (PT) have the largest piezoelectric coefficients ever reported. Many possibilities of chemical substitutions in the perovskite lattice offer wide possibilities of tuning physical properties relevant to the technological applications.

The electromechanical properties of $PbMg_{1/3}Nb_{2/3}O_3$-$0.17PbTiO_3$ (PMN-17PT) single crystals will be reported in this contribution. PMN-17PT composition is below the morphotropic phase boundary (MPB) but it still possesses quite high electromechanical constants. This material can be suitable for the soft piezoelectric applications. The origin of piezoelectricity will be discussed in these crystals.

Another studied system is a ternary solid solutions consisting of sodium bismuth titanate (NBT), strontium titanate (ST) and lead titanate. The relaxor part of the solid solutions is the 0.4NBT-0.6ST. Lead titanate can exchange both of the components of 0.4NBT-0.6ST solid solutions. The compositional dependence of electromechanical properties will be presented. The comparison between the two different relaxor-PT systems will be also discussed.

PO-81

Dielectric Properties of $BaTiO_3$ Based Composites

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In the last few decades there has been a growing interest in lead free piezoelectric materials. The main driving force is limitations due to environmental concern. The most well-known example is 2003 European Union’s RoHS (Restriction of Hazardous Substances) directive, which has limited the use of lead in certain fields [1]. $Pb(Zr_xTi_{1-x})O_3$ (PZT) is the most commercially viable piezoelectric material due to its high piezoelectric constant, ability to operate in a wide temperature range [2]. Unfortunately, it is lead-containing, thus falls under the restriction of RoHS.

In our presentation broadband dielectric properties of $BaTiO_3$ (BT) based composites with core-shell structure in temperature range of 100 to 500 kelvins will be presented. The composites were prepared in two steps. BT, $BiFeO_3$ (BF), $BaTiO_3$-$Bi(Mg_{0.5},Ti_{0.5})O_3$ (BT-BMT) and $BaTiO_3$-$Bi(Mg_{0.5},Ti_{0.5})O_3$-$BiFeO_3$ (BT-BMT-BF) nanoparticles were compressed with TiO_2 (ratio 1 : 1) in to low density pellets. Further, disk-shape pellets were submerged into barium hydroxide ($Ba(OH)_2$) for solvothermal solidification. In the end we obtain BT around BT, BF, BT-BMT and BT-BMT-BF particles. In such systems cores are stressed by barium titanate shell creating similar conditions as in morphotropic phase boundary (MPB), thus increasing dielectric and piezoelectric constants. We have investigated dielectric properties in broad frequency range of 4 different composite systems where core is a good dielectric, a relaxor, a ferroelectric and a non-ferroelectric material.

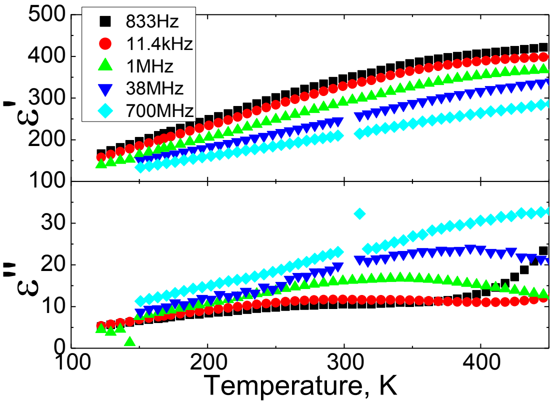

Fig.1 Temperature dependence of real and imaginary parts of dielectric permittivity for $Bi(Mg_{0.5},Ti_{0.5})O_3$-$BiFeO_3$

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PO-82

Dielectric Response of ZIF-90 and UiO-66 Metal-Organic Frameworks Under Different Gas Atmospheres

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Metal-organic frameworks (MOFs), also known as porous coordination polymers, recently have emerged as a new class of crystalline porous materials which has attracted a vast attention of the scientific community. The ability to vary the size and nature of MOF structures without changing their underlying topology, ultrahigh porosity, high thermal and chemical stability are very promising for gas adsorption and storage, molecular separation, catalytic purposes, water harvesting and etc [1-2].

We have investigated dielectric response of ZIF-90 and UIO-66 MOFs, prepared using a novel water-based synthesis procedure [3], under N_2, CO_2, CH_3OH, water vapour atmospheres and vacuum in wide temperature and frequency ranges. Analysis of measured complicated dielectric spectra allowed us to distinguish several relaxation processes caused by lattice and adsorbed polar molecule dynamics. Temperature evolution of these relaxation processes and influence of surrounding gas atmosphere was analysed in order to establish gas sensing abilities of these MOFs.

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PO-83

Dielectric Properties of PVDF-based Barium Titanate and Nickel Zinc Ferrite Flexible Films

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Flexible ceramic-polymer composites are perspective flexible electronic components due to the possibility to combine mechanical flexibility with the remarkable electrical and/or magnetic properties such as high dielectric permittivity, good magnetic and piezoelectric properties, etc. [1]. Polyvinylidene fluoride (PVDF) is one of the frequently used electroactive polymer due to its excellent flexibility, chemical resistance and tunability. Inclusion of ferroelectric and ferrite fillers in the PVDF might give rise to a multiferroic state which would be attractive for multifunctional devices.

Here we report the dielectric studies of PVDF-based composite with $BaTiO_3$ (BT) and $Ni_{1-x}Zn_xFe_2O_4$ (NZF) obtained by hot pressing method. The BT and NF powders were prepared by the auto-combustion method [2]. These composites were embedded into a PVDF matrix under the defined and optimized pressure and temperature. The thickness of the flexible films was around 50 microns. The electrical properties of all flexible composites were measured in the cooling regime from 420 K down to 120 K temperatures. Silver contacts were evaporated on the flat surfaces of flexible films and the complex dielectric permittivity was calculated form the measured capacitance and loss tangent employing the flat capacitor method.

Obtained results have shown that the main dispersion in all the samples originates from PVDF matrix [3] but both BT and NZF alters the dielectric dispersion. Increase of BT content leads to increase of the dielectric permittivity in all temperature range. Thus it is clear that fillers can effectively tune the value of the dielectric permittivity in these films.

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PO-84

Non-Linear Dielectric Spectroscopy of Mn-doped $PbMg_{1/3}Nb_{2/3}O_3$-0.1$PbTiO_3$

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Relaxor ferroelectrics (RFs) are a specific type of polar dielectrics. The definition of RFs is associated with exceptional properties of this group of materials. That is, a broad and usually enormously large peak and a strong frequency dispersion of dielectric. The dielectric anomaly is not connected with any macroscopic structural change. Yet, solid solution of RF and ferroelectric may have an occurrence of actual structural phase transition. A good example is $PbMg_{1/3}Nb_{2/3}O_3$-0.1$PbTiO_3$ (PMN-0.1PT). However, the occurrence of structural phase transition in PMN-0.1PT is in debate. Mn doping of PMN-0.1PT is expected to produce pinning of polar nano regions (PNRs) of RF is probable, as well. A good tool to detect an changes of dipolar motions is non-linear dielectric spectroscopy. In case of RFs, third order susceptibility (χ_3) have positive anomaly in temperature range of anomaly of χ_1.

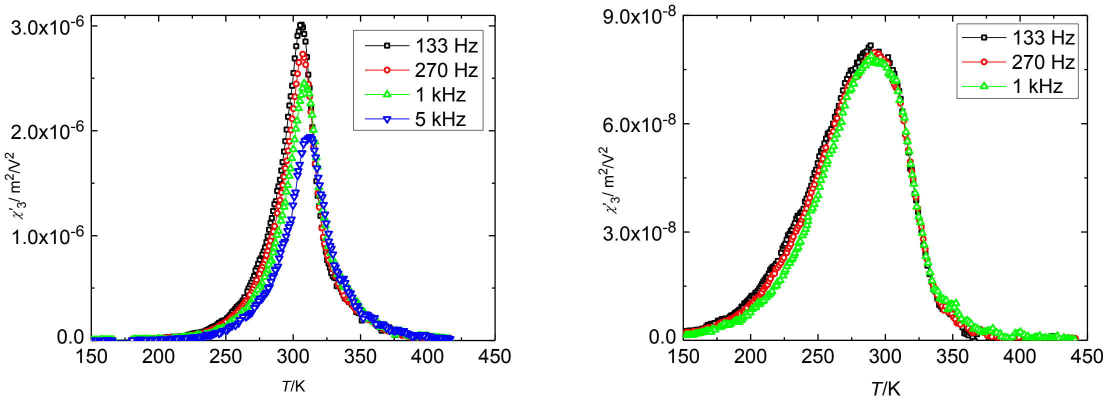

Figure 1. Temperature dependences of χ_3 of PMN-0.1PT (left) and PMN-0.1PT:1%Mn ceramics

In this work we conducted non-linear dielectric spectroscopy on PMN-0.1PT undoped, doped by 0.5% of Mn and 1% of Mn ceramics. Figure 1 shows, that $\chi_3(T)$ of 1% Mn-doped PMN-0.1PT has basically no temperature shift of maximum, as well as significantly decreased maximum value of χ_3. It may be, that such behavior is related to pinning of PNRs by Mn-doping: pinned PNRs are static and do not give contribution to collective motion of dipoles within the material. Further analysis and conclusions will be presented.

PO-85

Dielectric Investigations of Bismuth Niobate Manganate Ceramics

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The simple perovskite $BiMnO_3$ has received huge interest due to the possible coexistence of ferroelectricity and ferromagnetism [1]. Multiferroic materials, in which electric and magnetic ordering coexist in a single phase, have attracted a lot of attention, as well as bismuth niobate manganate.

In this work we present broad band dielectric spectroscopy results obtained for bismuth niobite manganate ceramics, $Bi(Mn_{1/3}Nb_{2/3})O_3$. Dielectric measurements were performed in wide temperature range (100 K – 500 K) at 20 Hz – 1 GHz frequencies. The distribution function of relaxation times $f(\tau)$ has been estimated from complex impedance spectra based on Fredholm integral equation:

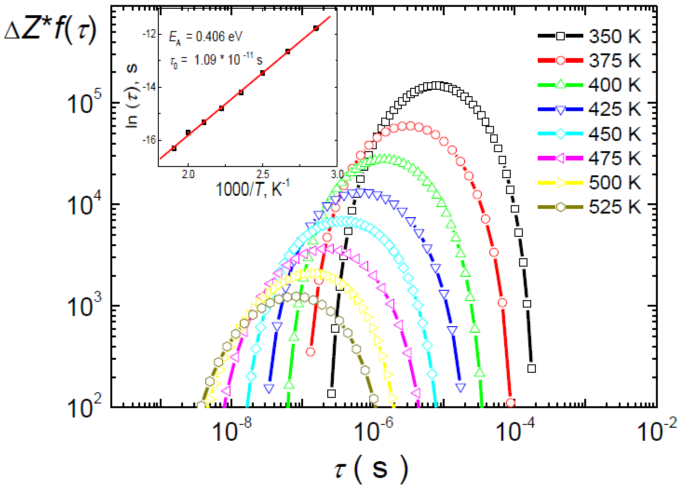

Fig.1 Distribution of relaxation times $f(\tau)$ of $Bi(Mn_{1/3}Nb_{2/3})O_3$ ceramics calculated at different temperatures from impedance spectra. Inset: the $1/T$ dependence of relaxation time for $Bi(Mn_{1/3}Nb_{2/3})O_3$ ceramics.
Solid lines are the best fit according to the Arrhenius law.

$$Z^*(\nu) = Z_\infty + \Delta Z \int_{-\infty}^{\infty} \frac{f(\tau) d\ln\tau}{1 + i\omega\tau}$$

The Tikhonov regularization method has been used [2]. The mechanism of electrical conductivity in $Bi(Mn_{1/3}Nb_{2/3})O_3$ ceramics will be discussed in presentation.

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PO-86

Ultra-low Percolation Threshold in Epoxy Resin – Onion-like Carbon Composites

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Composites based on an organic matrix filled with electrically conductive filler have raised the interest of many researchers during the last decades because of the possibility of getting lightweight conductive materials. This situation occurs as soon as the filler content exceeds a critical value called percolation threshold [1]. As a consequence, the resultant "synthetic metals" may have applications in the field of sensing or electromagnetic shielding, for instance [2].

In the present work, composites based on epoxy resin and onion-like carbon (OLC) were prepared and investigated. The measurements were carried out in a very broad range of frequencies (20 Hz – 34 GHz), and the results show that the percolation threshold in these composites is related to the size of the OLC aggregates, the biggest aggregates leading to the lowest threshold (0.7 vol. %). The observed critical exponent reasonably agrees with the theoretical value.

Composites comprising 10.89 vol. % of 250 nm-big OLC aggregates exhibit dielectric permittivity as high as 60 000 and electrical conductivity as high as 0.05 S/m at 20 Hz (Fig. 1).

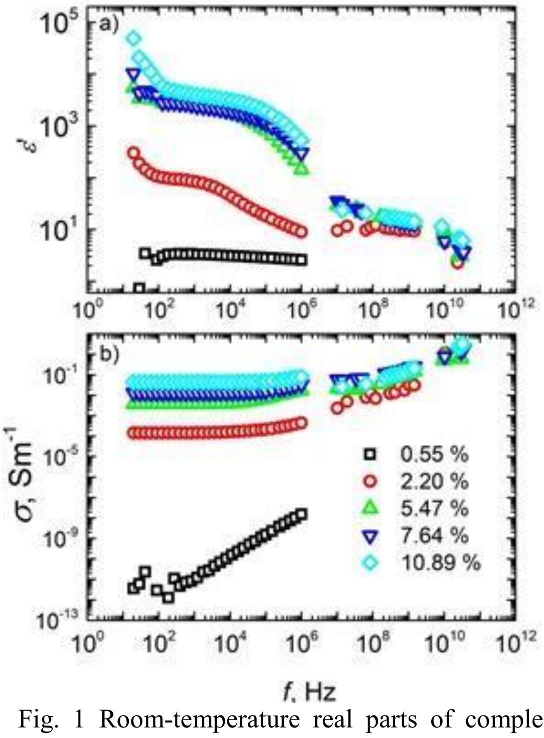

Fig. 1 Room-temperature real parts of complex dielectric permittivity and electrical conductivity of epoxy-based composites filled with OLC aggregates of average size 250 nm, plotted as a function of frequency.

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PO-87

Electrical Properties of Onion-like Carbon Composites

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Polymer-based composites presenting electrical percolation have attracted much attention because of the possibility to apply them as electroactive, sensitive materials, or as electromagnetic coatings [1]. It is an important to reach as-low-as possible percolation threshold in order to maintain the mechanical properties of polymers and to save the cost of expensive fillers. Onion-like carbon (OLC) as a composite filler has many advantages such as low cost, easy preparation and strong absorbtion of electromagnetic waves which leads to a potential applications for electromagnetic shielding.

In this contribution composites containing different OLC average sizes 40 nm, 100 nm and 250 nm were investigated. The electrical measurements were performed in broad frequency (20 Hz – 3 THz) range. In a frequency range 20 Hz – 1 MHz complex dielectric permittivity was measured at temperatures from 30 K to 500 K.

It was observed that the percolation threshold in composites strictly depends on OLC aggregate size. The electrical conductivity in the composites is mainly due to electron tunnelling between OLC clusters and quasi-one-dimensional hopping inside the clusters. In this presentation the impact of OLC aggregate size on broadband electromagnetic properties and the percolation threshold will be disscused.

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PO-88

Influence of Aluminosilicate Hollow Microspheres on the Electromagnetic Properties of MWCNT / PLA Composites

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Polymer composites embedded with nanocarbon inclusions attract scientists' attention around the world for a long time. This is due to a number of specific properties that nanocarbon fillers can provide for a pure polymer matrix, for example high electrical conductivity [1]. Electromagnetic properties of nanocarbon based polymer composites can be tuned by varying the type and amount of filler, leading to a wide range of permittivity, permeability and therefore electromagnetic response. In this study, we proposed to adjust the electromagnetic properties of a polymer matrix, namely polylactide (PLA), by adding aluminosilicate hollow microspheres [2].

By keeping constant the concentration of multiwall carbon nanotubes (MWCNT) inside the investigated PLA composites, we prepared samples with different concentration of aluminosilicate hollow microspheres, not exceeding 30 wt. %.

After dispersing the spheres into a mixture of PLA and carbon nanotubes, the final samples were obtained by hot pressing to ensure homogeneity and allowing the complex permittivity calculations by standard method (see [3] for calculation details).

The frequency and concentration dependencies of real and imaginary parts of permittivity were obtained using dielectric spectroscopy in microwave frequency range.

We demonstrated that under certain conditions it is possible to obtain a high value of the absorption coefficient (almost perfect absorption) in composites under study.

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PO-89

Synthesis and Studying of Reduced Few-Layered Graphene Coatings in Gas Sensor Applications

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Soon after discovery in 2004 the graphene have attracted much attention as potential material for gas/vapour sensors due to his variety in structures, gas sensing performances, room-temperature working conditions and tremendous chemical and mechanical stability.

In this work reduced few-layered graphene (rFLG) nanoparticles were synthesized using electrochemical pulse exfoliation method and waste graphite ingots. The regular change in voltage polarity in the synthesis process ensures both the separation of graphite in layers and the reduction of graphene oxide. A method for synthesizing rFLG and nitrocellulose (NC) composite film has been developed. Film formation method involves creation of suspension from rFLG, NC and acetone, applying the suspension on aluminium foil and drying, separation rFLG-NC film from aluminium. It has been observed that a successful synthesis of composite coating is possible with the mass ration of rFLG:NC at least 9:1 of which resistivity is on the order of $\approx 10\ \Omega\cdot\text{cm}$ in dependence from temperature and surrounding atmosphere. Sensor electrode was prepared by a simple dip-coating method and the response to humidity, acetone vapours and ammonia was measured and conclusion made that rFLG-NC coating is sensitive to many kinds of gases (cross-sensitive) what may result in false detecting or can be used to multi-sensor chips for artificial olfaction devices. However, till now, the mechanism of gas sensing based on graphene nanomaterials is not very clear, and different defects introduced (carbon vacancy, edge of layer, impurity atoms) to explain adsorption and reduction of specific gas molecules [1]. Nevertheless the future of graphene thin film gas sensors looks bright especially due extended lifetimes for a wide range of environments and applications.

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PO-90

Frequency Modulations in Electrochemical Exfoliation of FLG Material from Recycled Graphite

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During our previous work we have observed good exfoliation of Few Layer Graphene (FLG) material in DC setup at pulsed polarity change upon gas formation on electrodes. Both equal electrodes and chemically inert support electrode can be used in our setup. After varied Ion solution, polarity duration changes, voltage peak variations and sonication of samples, we have found that modulation of exfoliation peak using high frequency (kHz) allows for different quality FLG material to be obtained. Topographical as well as electrical characteristics are presented in this work. Powder type material synthesis to suspensions to thick films technological schematics as well as synthesis regimes discussed and previous work referenced in finalized

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PO-91

Mathematical Modeling and Parameter Optimization of the Enzyme Power Source for a Nano Drug Delivery System

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The research focused primarily on the heterogeneous nature of biological systems such as blood plasma and power sources of an enzyme based Biological Fuel Cells (BFC) viscous nature. Continued interventions to promote patient health include reliable and safe power sources for medical devices such as pace makers and drug delivery modules coupled to in vivo power generating nano-devices fuelled by readily available chemical energy sources and enzymes in the human body. With attention on efficacy, choice of safety materials and foreign body elimination is prioritised. To overcome a problem of systemic dosing and circulation, where drugs dosage is diluted without the option The kinetics associated with mobilising the drugs to the affected areas will require energy and electromagnetic control phenomenon's to ensure the target areas are reached and treated. Optimizing the power density control mechanisms essential in these biological systems applications such as stationary power sources as opposed to mathematically modeling and analysing the BFC to eventually optimize the performance using the machine learning approach we attempt to integrate the control mechanism in the instance of high and low fuel levels. In order to achieve this, model assumptions needed to be set in place with sensitivity to chemical and gaseous stimulus levels. The proposed model includes the introduction of a Distribution and Uniformity Factor (DUF) system with a theoretical understanding of effective uniform distribution of relatively dense viscous matrices and other immobilized synthetic by-products. Interpretation of the DUF system will allow scientists to rank the efficacy of an in vivo powered diagnostic and drug delivery system.

PO-92

Nafion and polyaniline composite modification with Li and Mg ions

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It is essential not only to reduce emissions but also to decrease air pollution already present in the atmosphere, such as CO2, in order to reduce the consequences of man-made atmospheric pollution. In the process of electrocatalysis CO2 can be reformed into fuels (CO, methane, methanol) or other hydrocarbons used in the chemical industry. It is essential to improve the properties of proton-conductive membranes for applications in electrocatalysis. .

In this work a research of Nafion-based membrane modified with polyaniline and ionic liquids was made. The goal of this work is to improve proton exchange membrane properties and research influence of ion liquid on composite properties. Composite membrane base is Nafion matrix with PANi 1 w% additive; after composite is prepared it is kept in different ionic solutions, for example, lithium and magnesium solutions. Li+ or Mg2+ ions could increase proton conductivity in composite polymer. Proton conductivity of activated and non-activated state and ions influence on composite properties are determined. This composition potentially allows achieving good proton conductivity at higher temperatures too. To define the best composition physiochemical properties of synthesized materials were determined by the means of thermogravimetric analysis, impedance spectroscopy, water absorption and its kinetics, and FTIR spectroscopy.

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PO-93

AlN Nanopowders as Luminescent Markers for Biological Materials

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Nanobiophysics is one of the fast developing field in natural sciences, where knowledge in nanosciences is applied to biological materials. Therefore a search of prospective nanomaterials, which could be used as luminescent markers for tracing the processes occurring in biomaterials, is in progress. Our previous investigations allow consideration that doped AlN nanopowder (NP) possesses the main properties necessary for realization of this task: *i)* a possible low toxicity of the material; *ii)* intensive and controllable luminescence within a convenient spectral region; *iii)* low cost of raw materials for nanostructure synthesis and accessible simple synthesis methods.

The present report is devoted to research of spectral properties of AlN NP doped with Tb and Mn in order to reveal their luminescence features. For this purpose AlN:Tb and AlN:Mn NP with grain diameter of $d \approx 60$ nm were used. Photoluminescence (PL) spectra and luminescence excitation (PLE) spectra were studied within a wide spectral region at room temperature (RT).

It was found that in both AlN nanopowder doped with Tb and Mn a strong luminescence with controllable intensity appears at 550 nm and ≈600 nm, correspondingly, which can be excited with ultraviolet light using the 263 nm laser.

In summary, we can conclude that luminescent AlN:Tb and AlN:Mn nanopowders are prospective materials for application as markers for biological materials.

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PO-94

Production of Variable Thickness Anodic Alumina Spacer for Metal-Insulator-Metal Optical Resonators

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Multilayer sandwich type systems, which consist of nanostructured and dielectric layers on reflective metallic substrate, attract considerable attention because they have potential features for producing refractive index sensors, enhanced scattering, and potentially useful for other optical applications [1,2]. Typically, the studies of multilayer systems with a tunable optical wavelength, require production of multiple samples with different layer thickness.

Here, we present a method for creating a multilayer structure with tunable resonant reflections at optical wavelength as a function of position on a wedge-shaped porous anodic alumina (PAAO). Desired PAAO thickness gradient was obtained using electrochemical oxidation (anodizing) of aluminum sheet while both anode and cathode were pulled out from the electrolyte solution at a preset withdrawal speed. The thickness variation can be observed as thin-film interference coloring (Fig 1.). The thickness variation from 50 nm to 1 μm and above could be achieved on the same sample. The thickness increased linearly with sample lateral coordinate while the nanopore diameter and separation remains intact throughout the sample [3].

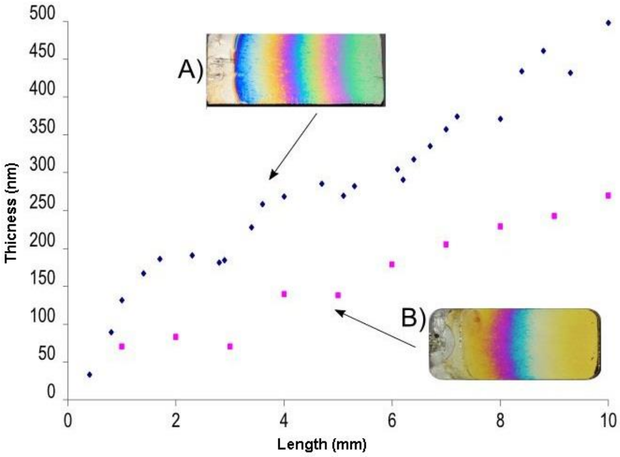

Fig. 1 The dependence of the PAAO thickness on lateral coordinate obtained at different withdrawal rates, A) 1,7 mm/min, B) 4,6 mm/min. The surface of the samples is covered with a 20 nm Au layer.

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PO-95

Up-Converting Nanoparticle Agglomeration Impact on Luminescence

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Luminescence based bio-imaging and in-vivo sensorics quickly gained popularity due to the various possible practical applications and advantages of the technology over conventional methods. One of the widely studied groups of materials is up-converting nanoparticles (UCNPs) with many research groups developing novel approaches to apply UCNPs for medical treatment and research. However, many technical difficulties and side factors are present in the approach. One of the problems already described in literature [3] but never studied in depth is the change of optical properties with unavoidable UCNP agglomeration.

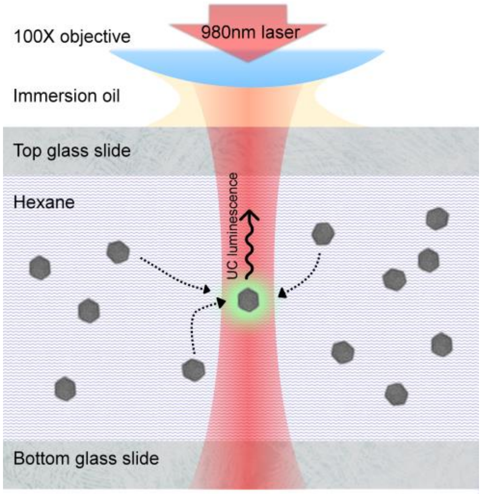

Fig.1 Schematic representation of optical trap used to obtain single nanoparticle spectral distribution

The present research is aimed to study the effect of agglomeration on the luminescence distribution. Spectrum from a single particle measured in optical trap was compared to a bulk sample as well as nanoparticles suspended in hexane. The study was performed using 50nm $NaYF_4$ UCNPs doped with rare earth ions (Er^{3+}/Yb^{3+}). By analyzing the red emission from the particles and correlating the output from the spectral detection system with observed CCD images it was found that the ratio between 653nm peak and 660nm peaks changes with the increase of the number of particles in the trap.

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PO-96

Thermostimulated Luminescence Properties of Neutron, Electron and Thermochemically-reduced $Y_3Al_5O_{12}$

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$Y_3Al_5O_{12}$, single crystals are known for their interesting properties such as high radiation-resistance, high melting point and high thermal conductivity. Consequently, they are candidates to several technological applications such as fusion energy devices and nuclear applications. Irradiation of single crystal $Y_3Al_5O_{12}$ in the reactor (i.e. fast and thermal neutrons and gamma radiation) produces many color centers (such as F-type center, interstitials [1-5] and many others) in the material. Similar defects are also formed by heavy ion irradiation or by fast electrons, while only electronic processes are important in the case of UV, X-ray and low energetic electron irradiation.

In this presentation we report the results of the thermostimulated luminescence measurements, performed between 300 and 720 K of the stored energy in $Y_3Al_5O_{12}$ single crystals, irradiated by fast neutrons with fluences of 2.1 x 10^{17} or 2.18 x 10^{19} n/cm^2, or also by 1.8 MeV electrons, or thermochemically reduced.

A clear pronounced dose effect was found and analyzed. In particular, four TSL peaks were observed in $Y_3Al_5O_{12}$ samples subjected 2.18 x 10^{19} n/cm^2, while in sample subjected 2.16 x 10^{17} n/cm^2 only three TSL peaks were detected. A comprehensive kinetic analysis of the glow peaks in $Y_3Al_5O_{12}$ is performed. As usual, each TSL peak is characterized by the appropriate activation energies, which both crystals are 0.8 – 1.3 eV. The obtained values are compared with the appropriate activation energies for F-type center annealing in neutron- and heavy-ion irradiated $Y_3Al_5O_{12}$ as well as also with similar TSL data for Al_2O_3 and $Y_3Al_5O_{12}$ [2-5]. Furthermore, we have also performed a comparative analysis of the photoluminescence properties of a series of neutron-irradiated and non-irradiated $Y_3Al_5O_{12}$ single crystals.

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PO-97

Cathodoluminescence Studies of Nanostructured AlN, AlN Nanotube/CsI Scintillator and AlN Nanotube/Polymer Composites

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Nanostructures of Aluminium Nitride (AlN) – nanotubes, nanowires and nanoparticles have been successfully synthesised by using a high temperature, highly non-equilibrium DC arc plasma method and investigated with different spectroscopy methods, including XANES, FTIR, neutron powder diffraction and inelastic neutron scattering [1-3].

Here we report the results of the cathodoluminescence studies of the AlN nanotubes and nanoparticles, which have been measured between 80 K and room temperature (RT) under electron irradition with 10 keV energy. Low-temperature CL spectra of nanostructured AlN have been compared with those of the commercially available AlN powder. The significant difference between emission spectra of the three investigated samples has been established. Commercial AlN has been found to emit a band peaked at 3.47 eV which is commonly ascribed to oxygen impurities. Emission of the AlN nanoparticles is centered around 3.66 eV while CL spectrum of AlN nanotubes show complex character with at least three peaks at 2.2, 3.0 and 3.5 eV in the photon energy range of 1.8 – 3.8 eV. CL intensity of the nanostructured samples has been found to decrease significantly at RT, most probably due to a combination of non-irradiative relaxations at the surface, electron-phonon interactions and the reabsorption of the emitted light. CL of AlN-nanotube/CsI-scintillator composites has been also studied. Energy transfer via luminescence emission from CsI scintillator to AlN nanotube is demonstrated. Luminescence properties AlN nanotube/polymer composites were also studied and compared with those obtained for AlN nanotubes and nanoparticles.

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PO-98

Influence of Pressure and Temperature on X-ray Induced Photoreduction of Nanocrystalline CuO

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Nanocrystaline copper(II) oxide (CuO) attracts much attention due to a wide range of possible applications, including gas sensors, catalysis, batteries, supercapacitors, field emission displays, nanoenergetic materials, photodetectors and solar cells [1]. Better understanding and optimization of device operations requires monitoring of their structure-functional property relationship under *in situ* and *in operando* conditions involving experiments with high-intensity synchrotron X-ray radiation. Under specific conditions, the incident X-ray beam may alter the conditions of the experiment and lead to changes in chemical properties of the sample. It is known that a reduction of metal ions in solution can occur upon radiolysis [2, 3].

In this study, we used focused synchrotron X-ray irradiation to follow kinetics of CuO photoreduction as a function of pressure and temperature (Fig. 1). We found that no reduction was observed for microcrystalline CuO. However, the rate of nanocrystalline CuO reduction increases upon (i) a decrease of the crystallite size down to nanoscale, (ii) an increase of temperature and (iii) at lower pressure.

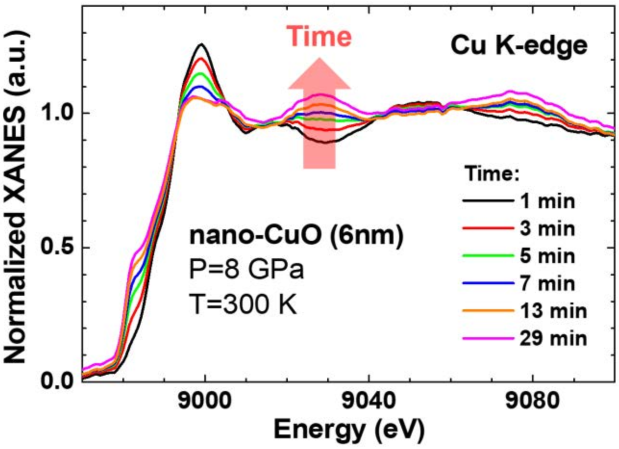

Fig.1 Kinetics of X-ray induced photoreduction of nanosized CuO (6 nm) at P=8 GPa and T=300 K as detected by the Cu K-edge XANES.

These findings are important for all studies dealing with high flux X-ray beams, in particular, in the case of nanosized CuO catalysts.

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PO-99

Investigation of Plasmon Properties of Cu Nanoparticles in Various Solvents

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This paper presents the results of an investigation of the influence of the solvent on the dimensional, structural and optical properties of Cu metal nanoparticles.

Nanoparticles of Cu were obtained by laser ablation method of a metal target in various solvents. The ablation of the metal target was carried out by the second harmonic of the solid-state Nd: YAG laser (SOLAR LQ 215, λ_{gen} = 532 nm, E_{pul} = 90 mJ, τ = 10 ns). In the process of obtaining a colloidal solution of Cu nanoparticles, deionized water, isopropyl alcohol, acetone, ethylene glycol, ethyl acetate were used, which differ in boiling point values. The concentration of Cu nanoparticles was determined from the change in the mass of the target before and after ablation. For Cu nanoparticles with laser ablation for 10 minutes, the concentration was $C=2{,}7\cdot10^{-4}$ mol/L. The size of Cu nanoparticles in colloidal solutions was determined by dynamic light scattering using of Zetasizer Nano ZS (Malvern) submicron particle size analyzer. The size of Cu nanoparticles in acetone is 107 nm, in ethylene glycol the average nanoparticle size is 11 nm. Based on the results obtained, it is established that when laser ablation increases with an increase in the boiling point of the solution, the average values of metal nanoparticles decrease.

The plasmon absorption spectra of Cu nanoparticles in various solvents have been researched. It is shown that the maximum absorption of Cu nanoparticles in isopropyl alcohol is located at a wavelength equal to 582 nm, the half-width of the spectrum corresponds to 78 nm. In ethylene glycol, acetone and water, the maxima of the absorption spectrum of Cu nanoparticles are located at wavelengths equal to 560, 580 and 650 nm, the half-width of the spectra is 86, 98, 100 nm, respectively. In the case of the absorption spectrum in ethyl acetate, the absorption maximum is observed at a wavelength of 580 nm, the half-width is 92 nm. It is established that the average sizes of Cu nanoparticles determine the position of the maximum of the plasmon absorption band of Cu nanoparticles.

PO-100

Synthesis and Applications of Dense Plasmonic Nanoparticle Arrays on Porous Anodic Alumina Templates

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We present a study of optical properties of dense noble metal nanoparticle arrays obtained using capillary force assisted colloid deposition on porous anodic aluminum oxide (PAAO) surfaces [1]. PAAO is a self-organized structure where pore diameters and center-to center distances can be selected by choice of anodizing voltage and electrolyte solution, such as oxalic or sulfuric acid. The nanoparticle size can be tuned during colloid synthesis and is independent from the PAAO morphology. This enables engineering of nanoparticle arrays with desired nanoparticle size and small interparticle gaps (Fig. 1) that are of interest for example in surface enhanced Raman spectroscopy. The high array density results in strong near-field coupling between neighboring particles at optical wavelengths. The arrays have short-range ordered structure, which results in complex electromagnetic field distribution in response to external radiation. Further, the interactions are sensitive to environmental changes and mechanical deformations. The arrays can be transferred to elastic membranes, which opens the possibility of applications for simultaneously probing the chemical composition, refractive index, and mechanical motion of samples brought in contact with the NP arrays.

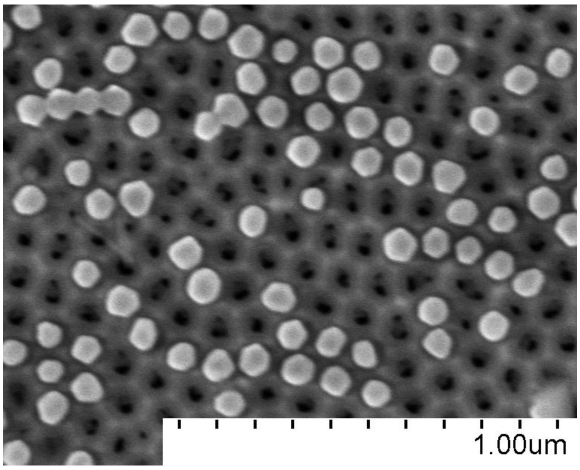

Fig.1 Array of 80 nm diameter Au nanoparticles deposited on oxalic acid electrolyte PAAO.

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PO-101

Properties of CaF_2 and BaF_2 Nanofluorides Produced by Pulsed Electron Beam Evaporation

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In this study multimodal mesoporous magnetic-luminescent nanopowders (NPs) of CaF_2 and BaF_2 with high defect density were prepared by pulsed electron beam evaporation [1] of nonmagnetic solid-state targets of calcium fluoride and barium fluoride. The produced NPs hold promise for application in spintronics, photonics, nanomedicine and other areas. The influence of annealing in air on the annihilation of color centers, magnetic, luminescent, textural and thermal properties of fluoride NP has been studied. The specific surface area of prepared BaF_2 and CaF_2 NPs reached 34.8 and 88.7 m^2/g, respectively. The magnetic properties of nanofluorides are strongly affected by both annealing temperature and storage time due to change in concentration of various types of defects (primarily F-centers). The high nonstoichiometry of NPs obtained by pulsed electron beam evaporation plays a major role in the formation of various structural defects in the studied nanofluorides.

The work was performed within the subject of the state task No. 0389-2015-0026 and partial support of projects of the Russian Federal Property Fund No. 18-08-00514. Magnetic measurements were taken within the state task on the subject MAGNET No. AAAA-A18-118020290129-5.

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PO-102

Some Features of Surface-Ligand Interactions in Nanosized Fe_3O_4 Probed by Colloid Magnetometry

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Surfactants play a vital role to enable solution processing of nanoparticles via a simple, easily scalable and highly versatile colloidal route. Carboxylic acids (e.g. oleic acid) are used extensively in the chemical synthesis and stabilization of nanomaterials based on metals and metal oxides [1]. However, the difficulty of exercising precise compositional control over the solutions produced by a chemical route obscures many aspects of the surface-ligand interactions.

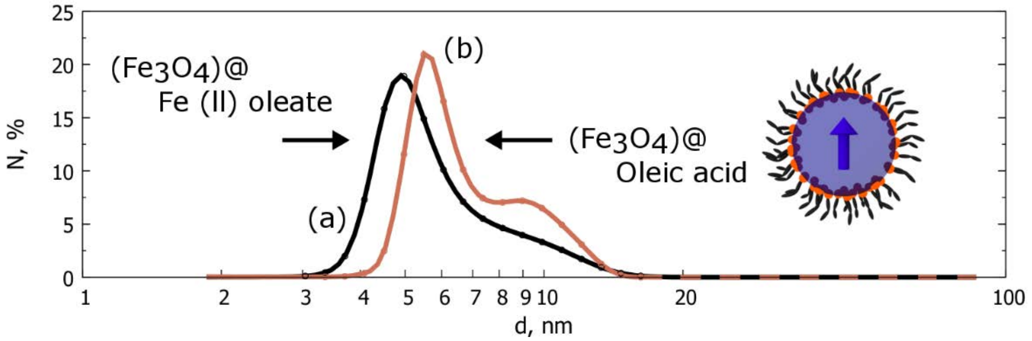

Fig.1 Results of magnetometric analysis: particle size distribution *(a)* – after treating with Fe^{2+} oleate, *(b)* – extraction by oleic acid.

Using electrodispersion of metallic iron in an aqueous environment without additional reagents we create a chemically clean model system based on nanosized synthetic magnetite [2] where the details of magnetic metal oxide - surfactant chemisorption can be studied by high sensitivity magnetic granulometry with nanometric precision.

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PO-103

ZnO/WS_2 Nanowire Core/Shell Heterostructures for Light Detection

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Potential applications of 1D and 2D materials in electronics and optoelectronics is a topical research subject due to the possible miniaturization of currently used devices and due to interesting properties, that materials exhibit in nanoscale. In recent years, transition metal dichalcogenide materials, especially WS_2 and MoS_2, have attracted significant attention due to their unusual properties, therefore offering numerous potential applications in optoelectronics, sensing and microelectronics [1], similarly to semiconductor nanowires [2]. As the surface plays an important role in nanoscale materials and, consequently, it has a strong influence on their properties, even a very thin coating can greatly improve optoelectronic properties of nanostructures by modifying the light absorption and spatial distribution of charge carriers.

To use these advantages, ZnO/WS_2 core/shell nanowire heterostructures with a-few-layers thick WS_2 shell were prepared. These nanostructures were characterized by scanning and transmission electron microscopy, X-ray diffraction and Raman spectroscopy [3]. A single-nanowire two-terminal photodetector devices were fabricated (*Fig.1*) by placing the heterostructure onto gold electrodes inside a scanning electron microscope [4]. The results show that a few layers of WS_2 significantly enhance photosensitivity in the short wavelength range and improve the photoresponse time of pure ZnO nanowires for almost two orders of magnitude.

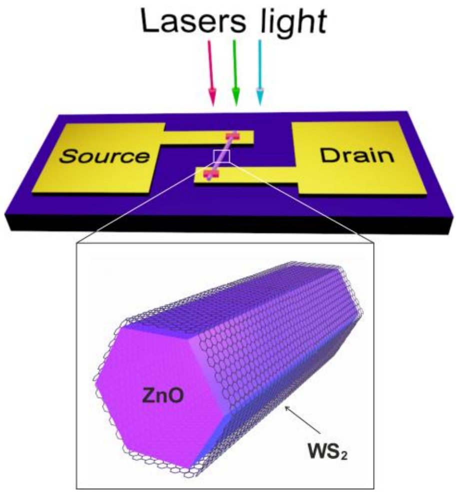

Fig.1 Schematics of ZnO/WS_2 core/shell nanowire-based photodetector

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PO-104

Influence of Inner Stresses on the Mechanical Properties of Fivefold Twinned Nanowires

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Finite element method (FEM) is a powerful research tool for many fields of physics and chemistry. This method can be also utilized in nanotechnology for studying and modelling mechanical properties and behaviour of nanowires (NWs). Attractive objects for this are, for example, noble metal NWs like silver (Ag) and gold (Au), due to their many potential applications, where they are under cyclical mechanical deformation [1,2]. These NWs have fivefold twinned inner structure with pentagonal cross-section [3]. This peculiar structure leads to the presence of inner stresses [4], which can have a considerable influence on the NWs mechanical behaviour.

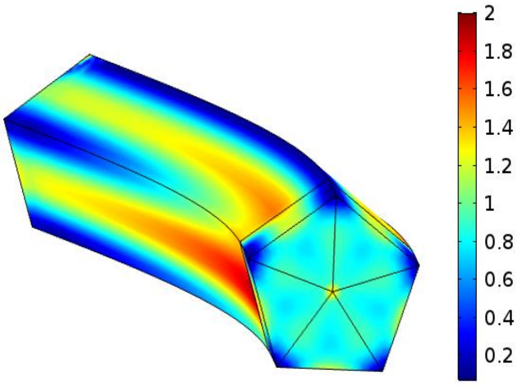

Fig.1 Von Mises stresses (GPa) in Ag NW during cantilevered beam bending test.

In the present work pentagonal Ag and Au NWs were modelled and their mechanical response simulated using FEM. The model takes into account the fivefold twinned structure and the presence of inner stresses. The cantilevered beam bending test was simulated (Fig.1) to further understand the influence of Ag and Au NWs structure on its mechanical behaviour. NWs with defects and distorted pentagonal cross-section were also simulated to compare the influence of the inner stresses in the cases of ideal and more realistic NW models.

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PO-105

Electronic Processes in Doped ZnO Nanopowders

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ZnO has excellent luminescence characteristics - especially fast intrinsic luminescence [1]. The luminescence spectroscopy is informative method for the doping process study in ZnO. The defect luminescence, excitonic (1LO_FEx), stimulated luminescence (SE) and electron-hole plasma (EHP) recombination were widely studied. At low temperatures the complex exciton processes take place. Donor-acceptor pair (DAP) luminescence can also serve as direct probe of the acceptors in ZnO.

ZnO NCs undoped and doped with Ir, In were prepared by solar irradiation by Heliotron reactor in Font Romeu, France [2]. Luminescence measurements were carried out with Andor Shamrock B-303i spectrograph equipped with Andor DV-401A-BV CCD camera. The x-ray excitation was used for radioluminescence spectra measurements.

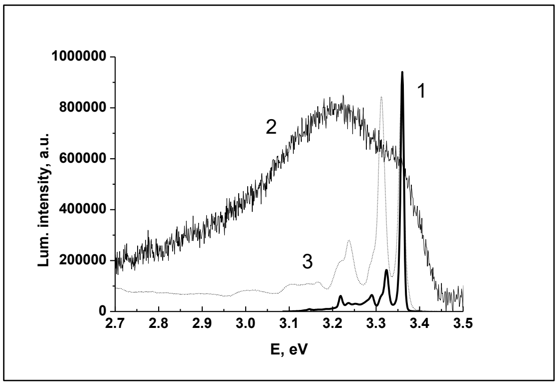

Fig.1 Radioluminescence spectra at 9K of ZnO single crystal (1) and In doped NC (3 wt%) (2) and Ir doped NC (3)

The decay of excitonic luminescence of ZnO is in subnanosecond time and therefore is prospective for scintillator application. The electronic processes in ZnO crystal, NC, coatings, ceramics are different and depend on doping concentration, intrinsic defects, electron/hole traps distribution. Fig.1 shows the luminescence differences of ZnO single crystal and doped NC. The present study is devoted to electronic processes of undoped and doped ZnO nanocrystals (NC).

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PO-106

Optical Properties of HfO_2 and $HfO_2:Eu^{3+}$ Synthesized by Various Methods

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Many modern applications like LED emitters and various scintillators require durable luminescent materials. These applications are often based on wide band gap materials doped with rare earth elements such as HfO_2 or ZrO_2 [1, 2, 3]. The wide band gap also ensures that the thermal quenching effects of luminescence are lower thus increasing the overall luminescence intensity [4, 5]. Besides promising optical properties hafnia is also a high-k material and has already been applied in various microelectronic devices [6, 7]. It is one of the most promising materials in the search for a replacement of SiO_2 [4] and an understanding of the structure and optical properties of the material provides a better understanding of the advantages and limits of HfO_2.

In this work, the optical properties of HfO_2 and $HfO_2:Eu^{3+}$ synthesized by using various methods and annealed at different temperatures are studied. The goal of this study is to explore the differences in optical phenomena when particles of the same size and dopant concentration have been synthesized by different methods. Photoluminescence studies are carried out to observe changes in luminescence intensity and spectral distribution. The amount of defects present is assessed via thermostimulated luminescence measurements. Time resolved luminescence and Judd Ofelt theory is used to determine the quantum efficiency and ion site symmetry.

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PO-107

The Dependence of the Morphological Properties and Intrinsic Defects of HfO_2 Nanoparticles on the Selected Chemical Synthesis Method

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A broad range of information about chemical synthesis methods of HfO_2 nanoparticles is available in the scientific literature, but there is no information available about studies in such field as the dependence of the morphological properties and intrinsic defects of HfO_2 nanoparticles in the chosen chemical synthesis method.

In this study, the samples of non-doped and doped HfO_2 nanoparticles were synthesized according to different chemical synthesis methods: sol-gel, combustion, precipitation, hydrothermal and molten salt method.

The morphological properties of the obtained samples were characterized by two different methods: powder X-ray diffractometry (XRD) and transmission electron microscopy (TEM). The XRD pattern shows that crystalline structures are monoclinic in all cases of the obtained non-doped HfO_2 nanoparticles. However, TEM results indicate that in some HfO_2 samples monoclinic crystallites are mixed with amorphous phases, as well as surface defects and different orientations of the crustal lattice were observed.

The first photoluminescence measurements shows that the intrinsic photoluminescence of non-doped HfO_2 samples depends on the chosen chemical synthesis method.

The influence on the morphological properties of non-doped and doped HfO_2 nanoparticles by using various chemical synthesis methods is further discussed.

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PO-108

Magneto-Gravitational Separation of Nonmagnetic Materials in Electronic Waste

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Separation of non-magnetic particles in a colloidal suspension of magnetic nanoparticles (a ferrofluid) is made possible by magnetic pressure exerted by the ferrofluid when in a magnetic field. A gradient of magnetic field will create a magnetic pressure imbalance, resulting in a magnetic force that enables magnetic levitation of non-magnetic particles. From balance of gravitational force and magnetic force, we can obtain an expression for density of material for which the floatation condition, effective density of material being equal to that of the ferrofluid, holds true:

$$\rho = \rho(ferrofluid) + \frac{\mu_0}{g} M|\nabla H|$$

To separate materials found in electronic waste, such as aluminum, copper and silver, it is necessary to achieve considerable values of both magnetic field gradient, which must also correspond to densities of every separable material at some point within the system, and magnetic induction, which should ensure saturation magnetization of ferrofluid for maximum efficiency – that corresponds to a field of $B = 0.4\ T$ or greater. Synthesis of appropriate magnetic nanoparticles to be used in the colloid can both ease the requirements for magnetic field configuration and improve economic efficiency of the waste separation method.

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PO-109

Carbon Aerogels as Nanomaterial for Supercapacitors

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The supercapacitors as the devices that use a high specific electric capacity of a double layer on the surface of the electrode in the contact with the electrolyte are widely used in modern technology. Naturally, to achieve high specific capacitance, a special organization of the electrode is required, and if activated charcoal is used in industry, the experimenters are now working with graphene-like nanostructures. However, in addition to the large capacitance, a low electrical resistance is required for the thick electrode to provide a small capacitor's ESR and large discharge current. High electrical conductivity can be achieved by creating an ultra-porous conductive matrix, which has led to a recent interest in aerogels as a material for electrodes.

Carbon aerogels are usually prepared by pyrolysis of inert precursors at temperatures of 700-1100 ° C; polymeric organic aerogels are used as the precursors. We investigated the dependence of the texture and electrochemical properties of carbon aerogels on the pyrolysis temperature of the original resorcinol-formaldehyde aerogels.

During the study it was found that the electronic conductivity of the samples increased linearly with increasing of pyrolysis temperature. It can be assumed that as the sintering temperature increases, the resistance of the grain boundaries between the aerogel particles decreases. The specific double-layer capacity in the sulfate electrolyte reaches 120 F / g and weakly depends on the pyrolysis temperature. The ESR of the electrode samples studied was about 15 Ohm for 5xd5 mm sample, but the obtained dependence allows us to modify the technology in order to obtain practically attractive parameters.

This work was supported by the Russian Science Foundation (Grant No. 18-13-00145).

PO-110

Mass Recovery of Carbonated Fabrics of Glass Fibres after Isothermal Heating

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The object of study was naturally carbonized Na-Al-Si glass fabric having a shell of differently oriented crystals of trona ($Na_2CO_3 \cdot NaHCO_3 \cdot 2H_2O$) on surface of glass filaments, that has a practical interest for fabric producers. Another motivation can be associated with the small sizes (below a µm in two directions) of crystals with increased attitude of surface to volume that facilitates the investigation of surface phenomena itself.

The samples of fabric were heated isothermally (up to 150-180^{0}C with a step of 5^{0}C during hour) and were measured mass decrease and its restoring at room temperature in different atmospheres as a function of time during a year or more. During heating there were observed the beginning of decomposition of trona as a mass decrease after 57^{0}C, or 73,5^{0}C. In a both cases after heating mass restores as sum of two exponents with different time constants (t) and mass constants (or pre-exponential factors) (A) (see relation in previous publication [1]), determined by regression technique. By using the different atmospheres of CO_2 and RH there are concluded that t_1 ($t_1<t_2$) and A_1 characterise physical adsorption of CO_2 and t_2, A_2- H_2O. The exponential mass restoring continues during at least of 15 min after heating, independently of preheating and beginning temperatures of decomposition. The steep adsorption increase of CO_2 (A_1) and H_2O (A_2) begins with start of decomposition of trona at 57^{0}C and 73,5^{0}C that could be caused by derive of new adsorption sites by degradation of crystals surface and increase its area. Up to 155^{0}C there are revealed three additional maximums of water adsorption for a case of decomposition with beginning at 57^{0}C.

There are discussed the decomposition of trona in dependence of preheating temperature and later mass recovery processes.

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We are grateful to State program of Latvia IMIS^2 for the financial support

PO-111

Wood-based Nitrogen Doped Activated Carbons for Fuel Cells

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Nowadays energy consumption constantly increases and development of effective and cheap electrochemical sources of power, such as fuel cells and electrochemical capacitors, is topical.

Power specifications and minimal price of H_2-O_2 fuel cells are limited by the expensive platinum-based catalysts, while prices of platinum increases while their reserves dwindle. Thus development of catalysts aimed to replace platinum-group metals is of the most important for the fuel cells design.

The main direction in development of non-platinum catalysts for the oxygen reduction is the study of cheap porous carbonaceous materials which can be obtained by the pyrolysis of polymers including renewable biomass. It is known that nitrogen atoms in carbon materials to a high degree determine properties of the doped activated carbons, such as high electrochemical stability, hardness, electric resistance, etc. The lack of sufficient knowledge on the doping of the carbon materials calls for the ongoing researches of properties and structure of modified carbon matrix.

Current study is devoted to highly porous activated carbons synthesized using alkali thermochemical activation from wood, cellulose and cellulose production residues – craft lignin and sewage sludge. Activated carbon samples were doped with dicyandiamide and melamine for the application as fuel cell cathodes. Conditions of nitrogen introduction (solvent, treatment temperature) and its content in the carbonaceous material, as well as porous structure characteristics, such as specific surface and pore size distribution, were studied.

It was found that efficiency of doping reaction depends on the elemental oxygen content in the activated carbon. Relationships between nitrogen content, porous structure characteristics and electrodes electrochemical properties are demonstrated.

Acknowledgments: The study was supported by M-ERA.NET project "Wood-based Carbon Catalysts for Low Temperature Fuel Cells (WoBaCat)"

PO-112

Characterization of Conductive PEDOT:PSS Films Blended with SWCNTs and PVA

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Conductive polymer poly(3,4-ethylenedioxythiophene):Poly(styrenesulfonate) (PEDOT:PSS), has reached attention as a perspective material for conductive polymer applications at the same time showing decent thermoelectric properties [1]. Single-walled carbon nanotubes (SWCNTs) can improve electrical junctions between PEDOT:PSS particles giving contribution to electrical conductivity and the thermopower improvement [2]. As PEDOT:PSS exhibit brittleness, that reduce its usage abilities, it was chosen to apply non-conductive polymer polyvinyl alcohol (PVA) to modify PEDOT:PSS.

The PEDOT:PSS/SWCNT composites were prepared by dispersing SWCNTs in the PEDOT:PSS solution by ultrasonic probe. For PEDOT:PSS/PVA/SWCNT preparation, PVA was added to PEDOT:PSS solution at the same concentration and stirred at 80 °C until the PVA was fully dissolved. Then SWCNTs was added in the same manner as previous.

Measurements of thermopower properties show that SWCNTs above 1 wt. % can improve Seebeck coefficient mainly by increasing electrical conductivity of PEDOT:PSS. As expected PVA reduced this property however at higher SWCNT concentrations (> 3 wt. %) it is still possible to maintain the increase in thermopower effect.

Apart from thermoelectric property measurements, PEDOT:PSS/SWCNT and PEDOT:PSS/PVA/SWCNT were characterized in respects to it mechanical, thermogravimetric and thermophysical properties to evaluate overall applicability of the developed composites.

Acknowledgement: Financial support in the framework of the ERDF project Nr. 1.1.1.1/16/A/257 is greatly acknowledged.

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PO-113

Characterization of Bi_2O_3 Film in Compound with $MnFe_2O_3$ Nanoparticles

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Conventional non-volatile memories are expected to reach their technical limit in the near future, therefore alternative possibilities are seeked [1]. Resistive switching is proposed as the basis for future non-volatile memories, combining the advantages of DRAM and Flash, but avoiding their drawbacks [2].

In this study, $MnFe_2O_4$ nano-particles were precipitated to planar Si(100) and TiN/silicon substrates by spin coating and covered with Bi_2O_3 by atomic layer deposition. $BiCl_3$ was used as bismuth precursor, the oxidizer was O_3. The $MnFe_2O_4$ nanoparticles were precipitated by several precipitation and filtering steps following heating and centrifugation cycles. Nanoparticles and nanostructures with film were characterized using X-ray fluorescence, X-ray diffraction and scanning electron microscopy. The Bi_2O_3 film was deposited to the substrate uniformly (Fig. 1). Vibrating sample magnetometer (VSM) results showed a hysteresis loop width of 50 Oe for $MnFe_2O_4$ nanoparticles as powder (Fig. 2). When combined with Bi_2O_3 films, we saw first implications of resistive switching behavior. Electrical characterization will be also reported.

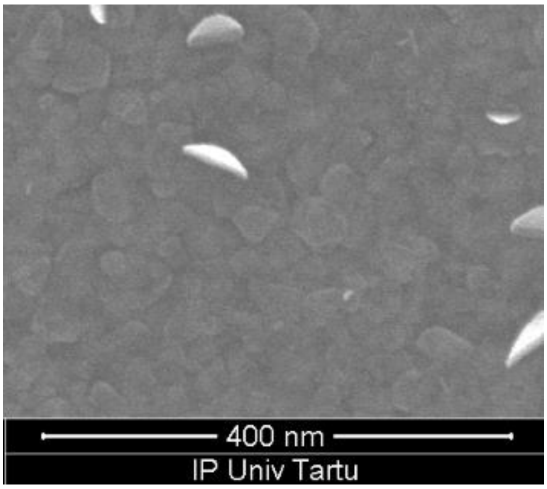

Figure 4: $MnFe_2O_4$ nanoparticles spin coated and covered with Bi_2O_3 using atomic layer deposition

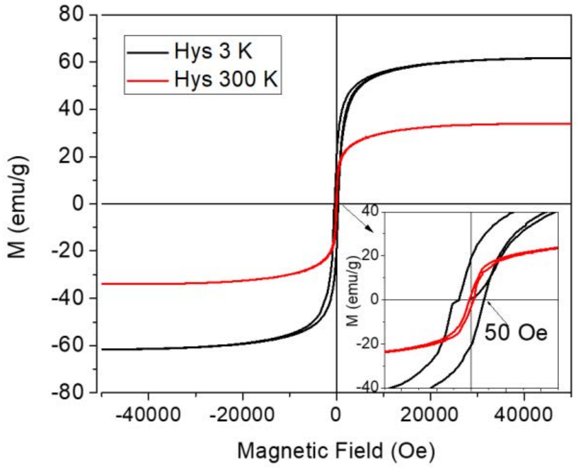

Figure 3. Magnetic hysteresis loops of $MnFe_2O_4$ nanoparticles as a powder measured by VSM at 3 and 300 K

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PO-114

Structural Studies of Y-doped Iron Thin Films

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Oxide dispersion strengthened ferritic steels (ODS FS) are promising materials for structural components in fusion reactors and other challenging applications. They often include yttria (Y_2O_3) nanoparticles. Preparation of ODS FS is a complex and expensive process [1]. Therefore, there is a search for alternative technological approaches, which can supply with easily accessible materials suitable for research activities. The use of magnetron sputtering technology is among promising methods.

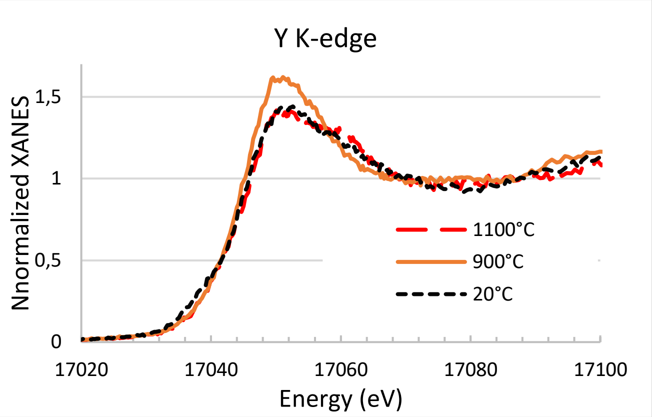

Fig. 1. Y K-edge XANES spectra of Y-doped (2%) iron thin films as produced (RT) and annealed to 900°C and 1100°C.

In this study, we have produced Y-doped (about 1-2%) iron thin films by DC magnetron co-sputtering of iron and yttrium metals at room temperature. The films were annealed in mixed argon-hydrogen atmosphere at different temperatures up to 1100 °C to simulate the ODS FS treatment process. Phase composition and morphology of the films were studied by X-ray diffraction, scanning and transmission electron microscopies. The local atomic structure around yttrium atoms was studied by synchrotron radiation X-ray absorption spectroscopy at the Y K-edge in fluorescence mode at ELETTRA synchrotron facility [2]. The analysis of X-ray absorption near edge structure (XANES) and extended X-ray absorption fine structure (EXAFS) revealed valuable information on the changes in the local environment and oxidation state of yttrium after different annealing treatments.

PO-115

TiO_2 Thin Films as Efficient Photocatalytic Material for Air Purification

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TiO_2 thin films fabricated by chemical spray pyrolysis method show air-cleaning properties comparable to nanopowdered materials. TiO_2 films are well adhered to the substrate and thereby additional risk to the environment by flying nanoparticles is eliminated.

Well adhered, highly transparent and highly hydrophilic (CA after UV treatment around 1 deg) TiO_2 thin films with a thickness of ca 250 nm were grown by chemical spray pyrolysis method onto a soda lime glass and boroslicate glass substrates. The films were deposited at various deposition temperatures in the range of 250 to 450 °C and annealed at 500 °C. All films consisted of anatase TiO_2 with the mean crystallite size in the range of 20 to 35 nm.

The films' photocatalytic activity for the degradation of VOC (methyl tert-butyl ether (MTBE)) was studied in multi-section plug-flow reactor. The process operating parameters, like air humidity, residence time, content of pollutants and irradiation source were varied. TiO_2 thin film deposited onto soda lime glass at 350 °C reveals the highest MTBE conversion rate of 81%. TiO_2 films deposited at 450 °C onto borosilicate substrate shows slightly higher MTBE conversion rate compared to the film deposited onto glass substrate due to higher mean crystallite size (anatase TiO_2 26 nm and 32 nm, respectively) and significantly lower Na content (0.5 and 7.5 at%, respectively) in the film.

PO-116

Hardness and Modulus of Elasticity of Atomic Layer Deposited Al_2O_3-ZrO_2 Mixtures, Nanolaminates and Al-doped ZrO_2

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Atomic layer deposition (ALD) is a technique to produce chemically and mechanically protective conformal thin coatings for various applications, micro- and nano- electro-mechanical devices or displays, for instance. The conformity ensures uniform deposition on complex details and parts.

In the present work ALD was used to deposit 100 nm of nanolaminates, mixtures of ZrO_2 and Al_2O_3, including Al doped ZrO_2, on soda lime glass at 300 °C. The relatively lower temperature of ALD (for instance, compared to regular chemical vapor deposition of 500 °C and higher temperatures) could allow to deposit the nanocomposites on materials which are mechanically sensitive to heat treatments, metal alloys for instance. The mechanical properties (elastic modulus, hardness) were measured by nanoindentation using continuous stiffness measurement technique [1,2]. The mechanical properties were compared to the thin film phase compositions examined *ex situ* for comparison.

The nanolaminates and amorphous mixtures showed higher hardness of 12 – 16 GPa compared to pure ZrO_2 (8 GPa) [3]. Pure Al_2O_3 had hardness of 14 – 16 GPa. Highest values, 16 – 18 GPa, were measured for thin films with cubic ZrO_2 in the structure. This could have been expected as the pure cubic form has the hardness around 20 GPa and it would enhance the performance of the thin film [4]. As an inconclusive result, ZrO2 could have orthorhombic I phase and including it gave some increased accuracy in phase composition calculation models, but announcing it was treated here with caution as the orthorhombic phase can be easily mixed up with tetragonal structure because both have similar single cell parameters.

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PO-117

Determining the Hardness of Thin Oxide Coatings

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In this work we studied the mechanical properties of thin corrosion resistant oxide coatings that were developed for aluminium alloys at the University of Tartu [1].

The coatings were made using anodizing the aluminium alloy substrates and sealing the pores by atomic layer deposition (ALD) with Al_2O_3, TiO_2, Al_2O_3/TiO_2 mix and Al_2O_3/TiO_2 laminate films [2]. The sealing by ALD was carried out with shorter and longer pulse times. The hardness of the coatings was measured by nanoindentation and the deformation marks were studied by scanning electron microscopy and cross-sectioning with focused ion beam.

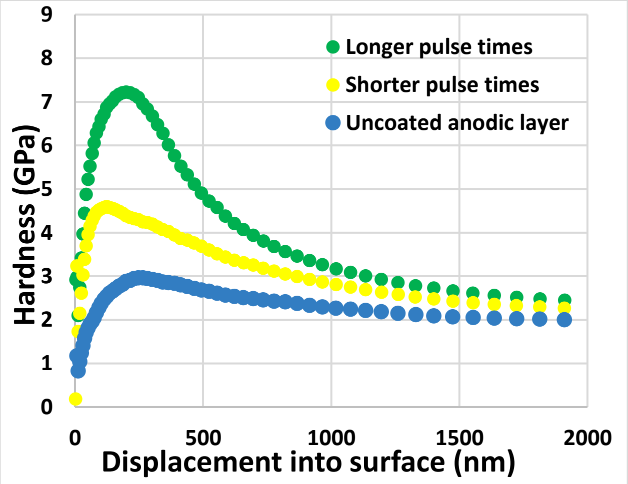

Fig. 5: Hardness of oxide coatings created by anodizing and ALD

The nanoindentation measurements showed that coatings made with longer pulse times were harder than the ones made with shorter times (Fig. 1). This was confirmed by SEM studies shown on figure 2, where the harder coating (Fig. 2 b) has fewer but larger cracks than the softer coating depicted on figure 2 a.

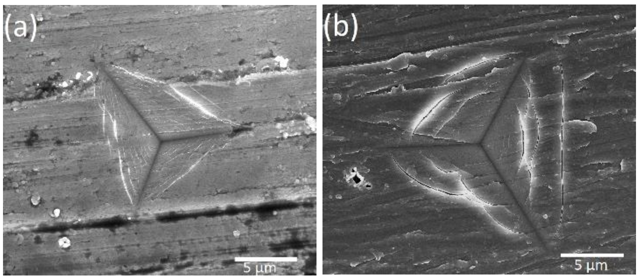

Fig. 6: SEM images of indentations on oxide coatings created by anodizing and sealing by ALD with short pulses (a) and long pulses (b).

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PO-118

Mechanical and Optical Properties of HfO_2/ZrO_2 Nanolaminates Grown Using Atomic Layer Deposition

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Hafnium dioxide and zirconium dioxide thin films grown using atomic layer deposition have high refractive indices, low absorption and good hardness, thus suitable for coatings in various applications [1-2].

Three laminates were deposited on Si and SiO_2 glass substrates using $HfCl_4$, $ZrCl_4$ and H_2O as precursors. Thicknesses of laminates were 105±3 nm, measured by spectroscopic ellipsometry on Si substrate. Laminates were also characterized using X-ray fluorescence, X-ray diffraction and scanning electron microscopy.

Extinction coefficients of laminate structures were close to zero in the wavelength range of 300-950 nm and refractive indices as high as 2.39 at 275 nm (Fig. 1). Monoclinic and tetragonal phases of HfO_2 as well as monoclinic and orthorhombic phases of ZrO_2 were observed (Fig. 2). Hardness measurements results by instrumented nanoindentation will be reported.

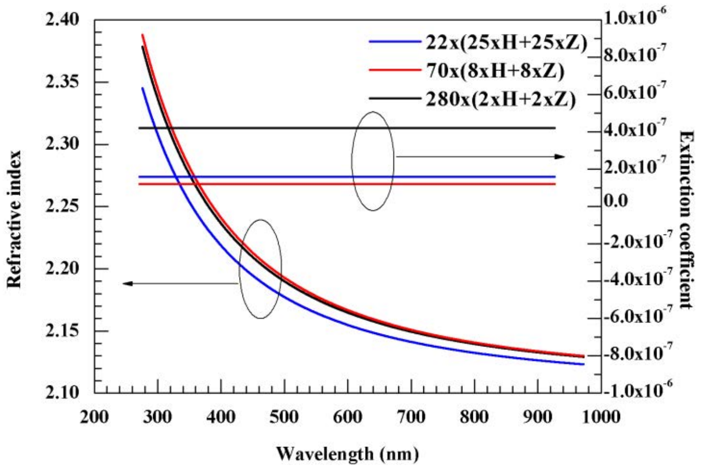

Fig. 2 Dispersion curves of laminates.

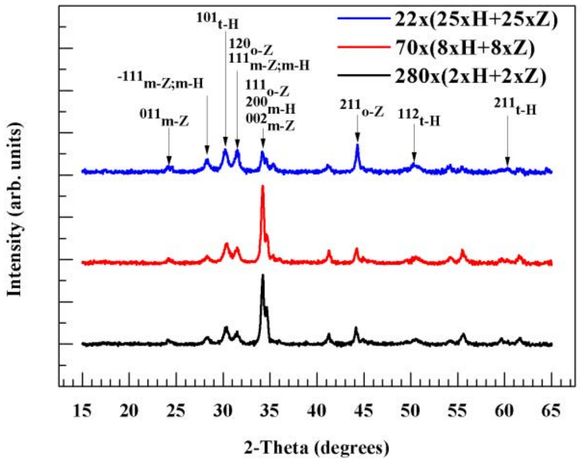

Fig. 3 Diffraction patterns of laminates. “H”, “Z”, “m”, “t”, “o” denote HfO_2, ZrO_2 and monoclinic-, tetragonal-, orthorhombic phases respectively.

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PO-119

Correlation between Technological Regimes and Microstructure for Nanogranular Ni-Fe Films

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Ni-Fe alloys have attracted much attention and are widely used for practical applications such as magnetic recording media, sensors, spintronic materials and magnetostatic shields thanks to optimal magnetic and functional properties. The properties of the Ni-Fe films are critically depend on the microstructure. The microstructure and the features of the crystal structure are determined by technological regimes of the film production and the film growth mechanism.

Ni-Fe nanogranular films have been formed onto silicon substrate via different electrodeposition regimes (direct (DC-regime) and pulse current with pulse duration from 1 s to 10 μs (long - LP, medium - MP and short pulse - SP regimes)) to investigate the correlation between technological regimes and microstructure. It has been demonstrated that limited number of nucleation centers, combined with low binding energy, resulted in the growth of large grains or “islands” by the Volmer–Weber mechanism for DC, LP and MP samples. As a result it leads to a rough defect film. The pulse duration of 10 μs (SP regime) was found to produce films with the average crystal size about 10 nm (fig. 1). We established that this grain size value for Ni-Fe films was a critical for transition to the nanolevel that limited the competition of the crystal surface energy and the interaction energy between initial atoms and substrate/film atoms. Thus for the SP deposition occurs by the the Stranski-Krastanov mechanism. So, with the transition to pulse-regimes and with a shortening of the pulse duration, deposited Ni-Fe films was found to be better in uniformity of the surface microstructure and thickness that provides stable mechanical and functional properties of the thin Ni-Fe films.

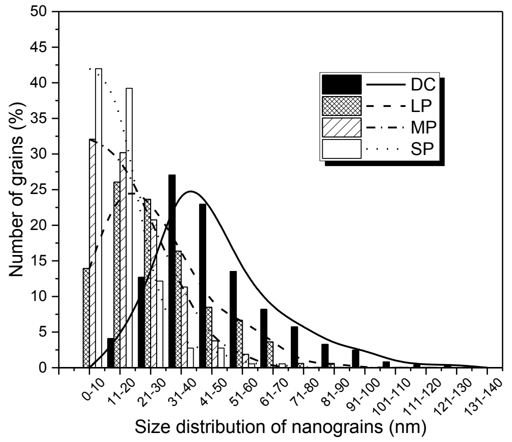

Fig.1 Size distribution and number of grains for different electrodeposition regimes.

PO-120

Specific Features of Magnetic Domain Structure in Epitaxial Ferrite-Garnet Films with Planar Anisotropy

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The interest in epitaxial Bi-substituted ferrite-garnet (FG) thin films deposited on oriented crystalline $Gd_3Ga_5O_{12}$ substrates (GGG) is due to the possibility of using them in various devices essentially based on their outstanding magneto-optic properties. As for the domain structure (DS) of uniaxial FG it was investigated in great detail during the last decades by many researchers; however, the studies of planar DS till now have received but scant attention.

In the present work we study the specific features of DS on (111) and (100) planes. It is shown that the magneto-optical figure of merit of the FG film working element depends on the perfection of its substrate. Substrate defects (dislocations, inclusions, slip bands, etc.) are inherited by the film, causing local changes in the magnetic properties. The results of studies of structural defects of bismuth-substituted ferrite-garnet epitaxial films are presented. Detailed examination of the DS response to the action of ac and dc external fields of varying direction was made. In given report we adduce a number of specific features of planar FG films not present in purely uniaxial films. Among these are ultralow coercivity values which may be used in highly sensitive magnetometric applications.

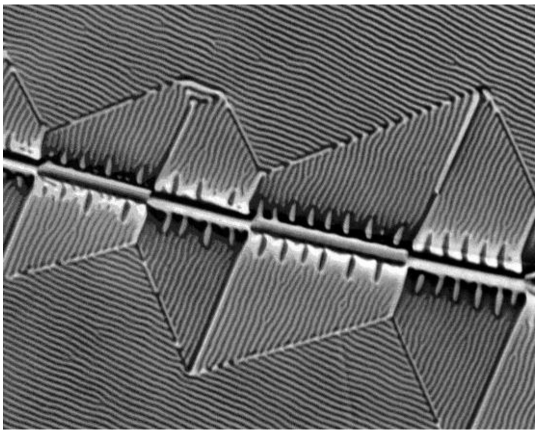

Fig.1 Scratch-modified domain structure of a ferrite-garnet planar film

In addition to Kerr and Faraday DS observations sclerometric (scratching experiments) were made to gain information on the effect of stress on the magnetic anisotropy of the material under study. A number of stress-induced DS peculiarities including a formation of complicated biperiodic DS were found to exist (Fig. 1).

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PO-121

Ferroelectric Properties of Composite Films Based on Polystyrene

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The work is devoted to the creation of composite materials of type 0-3 based on polymers with ferroelectric filler. Polystyrene was chosen as a matrix for composite films, ferroelectric ceramics PZT as filler. Polystyrene $(C_8H_8)_n$ with particle size < 2 μm was used. The ferroelectric ceramics were ground to a particle size of not more than 4 μm. The resulting PZT powder was introduced into a mixture of polystyrene and toluene in the following volume percentages: 10, 20, 35 and 50 %. The mixture was rolled on a fluoroplastic substrate and dried at room temperature in a fuming board until the mass loss stopped completely. The thickness of the composite films was 60-100 μm.

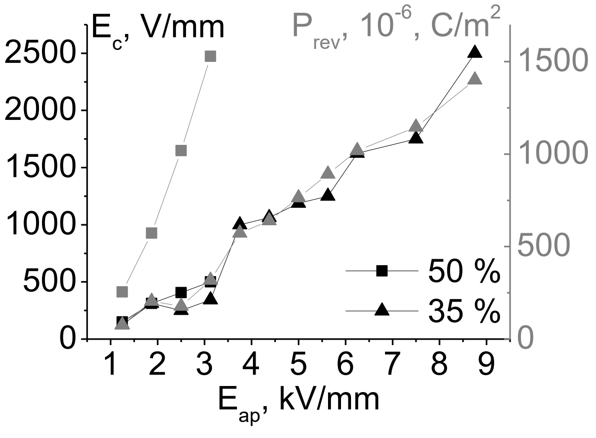

Fig.1 Dependence of the coercive field and reverse polarization on the applied field intensity for composite films with a filler content of 35 and 50%.

The temperature dependence of the dielectric properties was studied for the produced films. The polystyrene matrix begins to soften at the temperature above 80 °C, which complicates measurements. It is shown that the introduction of the filler increases the permittivity of the films in direct proportion to its concentration. It is also found that the permittivity does not depend on the frequency of the electric field in the frequency range from 10^{-1} to 10^{6} Hz. There is no one-to-one dependence of the dielectric losses on the frequency and concentration of the filler. It reflects the properties of the ferroelectric filler, the polymer matrix, and their interaction. The ferroelectric properties of films depend on the filler fraction. Thus, the films with a 10% PZT content have no dielectric hysteresis loops. With increasing concentration of filler there is an extension of the dielectric hysteresis loops and their area increases. The parameters of the obtained dielectric hysteresis loops as a function of the applied field intensity are shown in Fig. 1.

PO-122

Local Structure and Valence State of IrO Nanocrystalline and Amorphous Thin Film

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In order to investigate, in this research, the local atomic structure, bounding characteristic and valence state of Ir atom X-ray absorption spectroscopy (XAS) technique has been applied [1] in addition to XRD, UV-Vis-NIR absorption and FTIR spectroscopy, Hall effect measurement and Thermoelectric measurement. Zinc-Iridium Oxide thin films were deposited on glass, Si, and Ti substrates by DC reactive magnetron co-sputtering at room temperature.

The obtained UV-Vis-NIR absorption bands are associated with iridium ions at different valence Ir^{3+}, Ir^{4+} and Ir^{5+}. For the XANES L-edge ($L_{2,3}$, $2P_{1/2}$ and $2P_{3/2}$ respectively) absorption profiles, the magnitude of the absorption intensity indicates the available vacant states in the d-orbital, and its magnitude is therefore proportional to the oxidation state of the absorbing atoms [2] Fig.1 depicts the XANES spectra for the Ir L_3-edge from the zinc-iridium oxide thin film. The distribution of energy positions is significantly larger for the higher oxidation state. We observe the oxidation state change of iridium ions in Zinc-iridium oxide thin films from 5+ to 4+ [3].

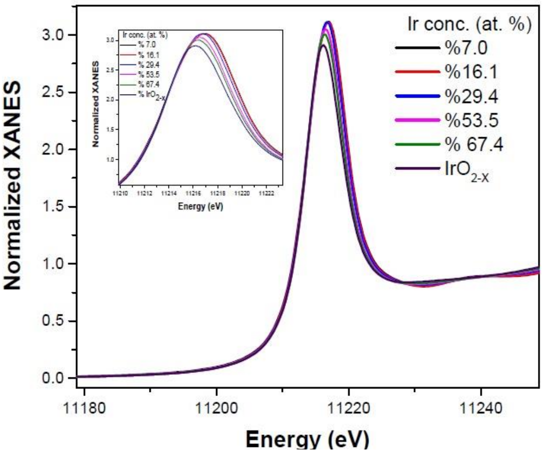

Fig. 1 Edge energy comparision of Ir atom with different Ir/Zn ratio

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Optical Properties of Zinc-Iridium Oxide Thin Films

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Transparent conducting oxides (TCOs) are metal oxides with high optical transmittance and high electrical conductivity [1]. Transparent conductive oxides (TCOs) of n-type have been extensively studied. Zinc oxides with iridium are a new class of p-type transparent oxide semiconductors [2]. The physics of iridium-based transition metal oxides has sparked significant interest because iridium oxide has many unique properties that make it an ideal material for applications as an emitter or protective coating material in field emission cathode arrays, used in vacuum microelectronic devices or as displays [3-5]. The results of investigation of the absorption spectra of zinc-iridium oxide thin films are presented. Zinc-iridium oxide thin films were deposited by reactive DC magnetron sputtering on various substrates [6]. Iridium concentration was controlled by iridium amount on the zinc target erosion zone and oxygen to argon ratio.

It is known that the iridium ions are present in different valences in many compounds. A very complex situation can occur where a certain ion in more than one valence state is present and in addition these ions occupy both tetrahedral and octahedral sites. The valence and site occupation of these ions is essentially determined by the growth conditions. It was found that the absorption spectra of zinc-iridium oxide thin films contain a broad bands in the visible (446 and 710 nm) and in near infrared (1100 and 3330 nm) region. At iridium concentrations between 40 to 60% a low intensity absorption band is observed in near infrared region at 1570 nm. The obtained bands are associated with iridium ions at different valence states Ir^{3+}, Ir^{4+} and Ir^{5+}.

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GeSn Optoelectronic Properties by Nondestructive Characterization

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Group IV elements of silicon and germanium have been served as basic materials for photo detection. Further extension of detection range to the mid-infrared region can be performed by few schemes. Among them, the all group IV alloy of germanium-tin (GeSn) based material has shown promising characteristics. Therefore we focused our study on optoelectronic properties of 400-nm thick $Ge_{0.96}Sn_{0.04}$ layers on silicon.

The main material parameters relevant for photo-detectors are carrier lifetime, diffusion coefficient and diffusion length. We employed contactless optical techniques as differential transmittivity, differential reflectivity, microwave photoconductivity and light induced transient grating for their nondestructive determination. The determined slow free carrier lifetimes by differential transmittivity were in 20-30 ns range (see Fig. 1) and weakly dependent on excitation, whereas differential reflectivity decays provided 0.5 ns decays attributed to Auger recombination and surface recombination (with ~ 1500 cm/s rate). Surface irradiation by 1064 nm laser for Sn redistribution by thermogradient effect did not induce appreciable changes of recombination parameters. Diffusion length of few μm was obtained, which verifies GeSn suitability for efficient photodetectors.

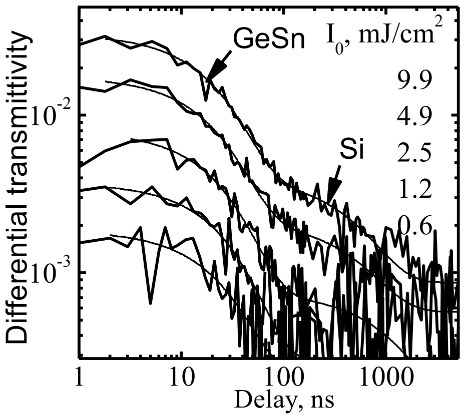

Fig.1 Differential transmittivity decays at different excitation fluences.

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Magnetron Sputtering of Zn/Al Target by High Power Pulses in an Ar/O_2 Atmosphere and ZnO:Al Thin Films Deposition

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Among transparent conducting oxides aluminium doped zinc oxide (AZO) is one of the most studied and used material due to the promising optical and electrical properties. Although high power impulse magnetron sputtering (HiPIMS) technology is a well-established thin film deposition technique, there are not a lot of scientific papers about TCO films deposition by the HiPIMS. In the HiPIMS regime ionized sputtered atoms could be used to control delivered energy to a growing film. The reactive sputtering is often used to deposit compound thin films; however, a precise process control is required because the desirable properties together with a sufficient deposition rate usually could only be obtained in the narrow reactive gas partial pressure range. The change in the current peak profile with the reactive gas could be used as a control parameter.

In this study the Zn/Al (98:2 wt.%) target was sputtered by rare high power pulses (power unit Melec SIPP2000) in an Ar + O_2 atmosphere. The profiles of peak current and the optical emission spectra collected 2 cm above the target surface were detected as a function of electrical parameters (frequency, pulse time, voltage) and oxygen flow. The set of AZO thin films without intentional heating was deposited by reactive HiPIMS and the film's electrical and optical properties were analyzed as a function of the oxygen partial pressure.

Plasma emission spectrum changes from mainly excited Ar emission to excited Zn emission when the frequency is decreased or the average power increased. The shape of the current peak changes significantly when an oxygen flow rate is varied. The resistivity in the range from 10^{-2} to 10^{-3} Ωcm was obtained together with the high visible light transmittance.

The results obtained in this study could be used to better understand and optimized the growth condition of AZO films by reactive HiPIMS.

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Comprehensive Characterization of the Amorphous Ta_xO_y Thin Films Deposited on Si and Glass

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Thin films of tantalum oxide (Ta_xO_y) are promising materials for application in modern nanotechnology. Thanks to the large values of dielectric constant and electrical resistance they have been applied as dielectrics in metal-insulator-metal memory devices, thin film capacitors for radiofrequency applications and metal-oxide-semiconductor transistors. The performed studies aimed to elaborate technology to apply them in a regenerable optical fiber biosensor [1,2]. The required material should be resistant to environmental threats or even play a role of protective coatings.

To be chemically robust, the material should be amorphous rather than in Ta_2O_5 crystalline form. Ta_xO_y may form nonstoichiometric materials, including suboxides, as well as over-stoichiometric compositions. Moreover, the crystallographic structure of Ta_2O_5 is still debated. The electrical, optical and chemical properties of the deposited materials depend on their composition and structure.The comprehensive characterization of films deposited on crystalline (Si) and amorphous (glass) substrates were performed with support of theoretical simulation.The XRD, XPS and XAS studies were performed on thin films deposited at the temperature of 100°C by atomic layer deposition (ALD) technique. Simulations were accomplished applying the density functional theory (DFT).

XRD confirmed the amorphous structure of the studied layers. The elemental composition, chemical shifts of elements and depth profiling studies were performed using **XPS**. The local atomic order around Ta atoms was estimated from analysis of **XAS** at L_3 Ta edge. The DFT calculations helped in interpretation of XPS data.

This work was partially supported by Interreg Baltic Sea Region Programme (Baltic TRAM), the EAgLE European project (FP7-REGPOT-2013-1, Project No. 316014), Polish Ministry of Science and Higher Education, Grant Agreement 2819/7.PR/2013/2, and as statutory activities at the Institute of Electron Technology and Institute of Physics PAS.

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PO-127

Studies of Thermoelectric Properties of P3HT for 3D Printing Applications

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3D printers are popular accessories both in industry and scientific labs and their industry is growing bigger by every day. People are looking for new ways and possibilities how to use them and what new opportunities could get out of them.

One of the possibilities where 3D printers could be used is printing of functional materials, which would possess not only geometrical/mehanical uses, but functional like thermoelectric ones aswell. Of unique advantages, 3D printing enables the generation of free-standing bulk objects, which are particularly useful for preparing thermoelectric material samples.

The main problem with those functional materials is ignorance about suitability for 3D printing process. Print and test procedure is not very beneficial, as costs for small amount of funcional materials are usualy high and certain amount of material is needed for test 3d printing, We are suggesting a series of experiments (annealing and melting) and mesurements of thin films with whom suitability of the materials for use in 3D printing is charachterised by mesuring their physical characteristics: electrical and thermal conductivity, Seeback coeficient and activation energies of the material.

In this work thermoelectrical properties of untreated and annealed (melted) P3HT and P3HT/F4TCNQ thin films will be shown and results discussed.

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XPS Studies of [EMIM][BF_4] Ionic Liquid Films

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Ionic liquids (ILs) are generally defined as molten organic salts with a melting point below 100 °C. These compounds have attracted great interest in the last few decades because of their uncommon physicochemical properties such as low melting temperatures, excellent solvation ability, relatively high thermal stability, low vapour pressure, non-flammability, high electrochemical stability etc. [1] One of the most powerful applications of ionic liquids is in supercapacitors, which have very high electrical power density and long life. Namely, by using ionic liquids instead of conventional electrolytes in supercapacitors one can increase their energy density substantially.

The behavior of ILs in several applications is determined by their electronic structure and interaction with substrates. The objective of the present work is a systematic study of the evolution of the electronic structure of ILs from ultrathin (including partly covered monolayers) to thick (bulk) films. By studying ionic liquid layers the XPS (X-ray Photoelectron Spectroscopy) data should be able to show what is the surface/interface influence on the ionic liquid electron structure.

Direct physical deposition has been used to iteratively deposit layers of [EMIM][BF_4] (1-Ethyl-3-methylimidazolium Tetrafluoroborate) on a Cu(100) substrate. The Cu(100) substrate was cleaned with several cycles of argon etching and annealing. The [EMIM][BF_4] ionic liquid (Sigma Aldrich, ≥99.0%) was vacuum dried and heated in the effusion cell for several days before deposition. After each deposition cycle XPS spectra were acquired with SES-100 hemispherical analyzer. A non-monocromatic Thermo XR3E2 X-ray tube was used with Al anode (Al Kα - 1486.6eV) at 200W source power.

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Photoluminescence and Electrical Properties of GaAs (111)A Epitaxial Layers Prepared by MOCVD

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In order to improve the performance of high-voltage diodes and transistors they are proposed on the base of GaAs epitaxial structures with crystallographic orientation (111)A. MOCVD technology for the formation of such layers significantly differs from that for GaAs (100) layers. Although one of the most responsible factors that affects properties of both types of prepared epitaxial layers is V/III element ratio in the gaseous phase. Formation of qualitative morphology of GaAs(111)A layers occurs at low crystallization temperature and high values of the V/III ratio [1], which significantly affects their properties.

Photoluminescence combined with electrical properties of GaAs (111)A layers are studied not enough. Therefore these properties of silicon doped GaAs (111)A/B and (100) layers obtained with different Ga and As partial pressures on substrates are investigated in the present work. It has been established that increase in the V/III ratio from 84 to 180 during the crystallization of GaAs (111)A layers leads to a significant change in photoluminescence spectra measured at temperature of 8 K. The near-complete fading of the bands with the maximum at 825 and 835 nm was observed because of dopants and complex donor-acceptor or acceptor transitions. GaAs (100) layers obtained under the same MOCVD technology characterized by a wide band with two peaks at 816 and 846 nm. Photoluminescence results suggest much more defects for GaAs (100) layers in comparison with GaAs (111)A/B. Formation of non-stoichiometric defects and their influence on the preparation of doped GaAs layers discussed in details. Obtained results might be used to prepare high quality GaAs epitaxial structure with crystallographic orientation (111)A.

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PO-130

Innovative Nanomaterials – Peculiarities of Formation of Strained Lead Selenide Nanolayers

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At keeping the strained state in $A^{IV}B^{VI}$ semiconductor nanolayers during a long period of time, there appears the possibility of flexible tunability of energy spectra of current carriers [1]. At doping these layers by impurities of variable valency, the uniformity of layers and a significant compensation of the concentration of current carriers are revealed additionally at stabilization of Fermi level deeply in the forbidden gap. The prospects of formation of high-temperature tunable lasers and high-speed and high-sensitive photodetectors in IR spectrum are opened. The implementation of such innovations is received at the development of modi-ficated technology of molecular epitaxy with “a hot wall”. At the example of lead selenide the character of strained layers growth on KCl. BaF_2 and NaCl dielectric substrates is analyzed. Two-stage growth of layers is revealed at the double influence of dislocations on its cha-racter. At the first stage the islands – nuclei emerged and merged and their surface-tension energy is transferred to dislocations and at the increase of the number of nuclei and as the result continuous growth of layers is accelerated. At the second stage of layer-wise growth, the elastic energy of layers increasing with the growth of thickness is enough for origination and acceleration of dislocations – the relaxation of strains takes place. The study of the inf-luence of the velocity of layer’s growth on formation of maximum deformations (tangential lattice constants) in connection with the interaction of nonstoichiometric defects is of interest. At the decrease of the thickness of layers lower than 100nm and of the growth velocity down to constant decimals nm/sec, the tangential lattice constant exceeds 6.200 Å , and the defor-mation is more than 0.015. At the mentioned growth velocities, the nonstoichiometric defects have time to annihilate in dislocation’s nuclei and cause the retardation of them. With the increase of deformation in layers, the texture of tetragonal phase is appeared in them. It leads to the appearance of additional narrow absorption band in optical spectrum not observed early in $A^{IV}B^{VI}$ semiconductors [2].

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