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Devoted to the 70th anniversary of birth
of Aleksey Vladimirovich Bushman
(16.10.1946–6.12.1993)

The book consists of the abstracts of plenary, oral and poster contributions to the XXXI International Conference on Equations of State for Matter (March 1–6, 2016, Elbrus, Kabardino-Balkaria, Russia). The conference is devoted to the 70th anniversary of birth of Aleksey Vladimirovich Bushman (October 16, 1946–December 6, 1993). The reports deal with the contemporary investigations in the field of physics of extreme states of matter. The topics are as follows: equations of state and constitutive equations for matter at high pressures and temperatures; shock waves, detonation and combustion physics; interaction of intense laser, x-ray and microwave radiation, powerful ion and electron beams with matter; techniques of intense energy fluxes generation; experimental methods of diagnostics of ultrafast processes; low-temperature plasma physics; physical issues of power engineering and technology aspects.

The conference is supported by the Russian Academy of Sciences and the Russian Foundation for Basic Research (grant No. 16-02-20029).

The editorial board announces with deep regret the death of the colleague and friend, Prof. Vladimir Grigorievich Novikov (July 4, 1950–October 2, 2015), who was a regular and active participant of the Conferences on Equations of State for Matter and Interaction of Intense Energy Fluxes with Matter starting with one of the first meeting.

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1. Equations of State for Matter

On mechanical measurements in high-energy-density physics

Fortov V E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

fortov@ihed.ras.ru

In this talk, actual methods and recent results of mechanical measurements in high-energy-density physics are reviewed.

A V Bushman and equation-of-state problem

Lomonosov I V

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

ivl143@yahoo.com

In thsi report, we'll present some details of A V Bushman biography, his scientific achievements and impact on equation-of-state (EOS) problem. Principal results include developing of multi-phase EOS for metals, their applications in numerical modeling of high-energy-density phenomena, systematization of reference shock-wave data. The current state of art and development of Bushman's approach on EOS problem are discussed.

Wide-range equations of state for compounds at high dynamic pressures

Khishchenko K V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

konst@ihed.ras.ru

An equation of state of matter over a wide range of pressures and densities is needed for analysis and simulation of physical processes under intense pulsed influences [1]. Accuracy of calculated results is determined mainly by adequacy of description of thermodynamic properties of materials in question. In the work, different approaches to modeling of equations of state for compounds after Bushman [2] are considered. A model of thermodynamic potential Helmholtz free energy with taking into account polymorphic transformations, melting and evaporation is presented. Based on this model, equation-of-state calculations are carried out for some alkali halides, oxides and organic compounds in a broad region of the phase diagram. Obtained results are compared with available data from dynamic experiments at high pressures.

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Atomic number scaling of electron spectra in semiclassical free atoms

Shpatakovskaya G V[1,@] **and Karpov V Ya**[2]

[1] Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, Miusskaya Square 4, Moscow 125047, Russia
[2] Bruk Institute for Electronic Control Machines, Vavilova 24, Moscow 119334, Russia

[@] shpagalya@yandex.ru

The atomic number scaling of the properties is known to be in the Thomas–Fermi (TF) statistical model. It means that the semiconsistent potential by the model may be calculated through the single function for all the elements. In the paper it is shown that one electron spectra of the free atoms in the TF potental exhibit the scaling properties too. The spectrum of the central potential with Coulomb singularity has been analysed in [1, 2]. It has been there shown that a screening of Coulomb potential leads to the energy deviation from the s-level $\varepsilon_{\rm nl} - \varepsilon_{n0}$ which quadratically depends on the orbital momentum $\lambda = l + 1/2$ (here n is a principal quantum number). We reveal the coefficients of the dependency have the atomic number scaling property and so an energy level ε_{nl} may be expressed through two "universal" functions $\epsilon(\sigma)$ and $\eta(\sigma)$

$$\varepsilon_{nl} = Z^{4/3}\epsilon(\sigma_n) + Z^{2/3}\eta(\sigma_n)\lambda^2, \quad \sigma_n = \pi n Z^{-1/3}. \tag{1}$$

We compare equation (1) results with the Bohr–Zommerfeld quantization condition ones. In addition we use the different screening functions: TF, Tietz [3] and Molier [4]. The comparison shows a rather good fitting of equation (1) for whole spectrum excluding a few upper levels.

This work was supported in part by the Russian Foundation for Basic Research (project No. 14-01-00828).

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Complex structures of dense lithium: Electronic origin

Degtyareva V F

Institute of Solid State Physics of the Russian Academy of Sciences, Institutskaya Street 2, Chernogolovka, Moscow Region 142432, Russia

degtyar@issp.ac.ru

Lithium—the lightest alkali metal—exhibits unexpected structures and electronic behavior at high pressures [1, 2]. As the heavier alkalis, Li is bcc at ambient pressure and transforms first to fcc (at 7.5 GPa). The *post*-fcc high-pressure form Li-$cI16$ (at 40–60 GPa) is similar to Na-$cI16$ and related to more complex structures of heavy alkalis Rb-$oC52$ and Cs-$oC84$. The other high pressure phases for Li ($oC88$, $oC40$, $oC24$) found at pressures up to 130 GPa are specific the only to Li. The different route of Li high-pressure structures correlates with its special electronic configuration containing the only 3 electrons (at $1s$ and $2s$ levels). Crystal structures for Li are analyzed within the model of Fermi sphere–Brillouin zone interactions [3, 4]. Stability of *post*-fcc structures for Li can be supported by Hume–Rothery arguments when new diffraction plains appear close to the Fermi level and characterized by pseudogap formation near the Fermi level decreasing the crystal energy. The filling of Brillouin–Jones zones by electron states for a given structure defines the physical properties as optical reflectivity, electrical resistivity and superconductivity. A necessary condition to understand complexity of structural and physical properties of Li above 60 GPa is assuming the valence electrons band overlap with the upper core electrons and increase the valence electron count under compression.

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Binodal layer and rarefaction shock in retrograde adiabatic expansion of warm dense matter in two-phase region of non-congruent phase transition

Iosilevskiy I L[1,2,@] **and Gryaznov V K**[3]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
[3] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] iosilevskiy@gmail.com

Remarkable feature of non-congruent phase transition (NCPT) is a more complicated structure of two-phase boundaries. Non-standard hydrodynamic behavior of warm dense matter (WDM) inside NCPT region is under discussion. In contrast to ordinary van-der-Waals-like transitions, thermodynamic path of adiabatic WDM expansion enters and leaves two-phase NCPT region at high enough entropies within so-called *retrograde scenario*. Two remarkable events result from this double crossing of phase boundaries when expansion is going within equilibrium (not metastable!) regime: (i) the *binodal layer* [1] ("plateau") appears when adiabatically expanding WDM enters two-phase region; (ii) rarefaction shock appears when matter leaves this region.
Features and parameters of both the events are discussed on the base of adiabatic expansion within two-phase NCPT region for chemically reacting WDM of high-temperature uranium–oxygen plasma of products of extreme accident heating of uranium dioxide [2].

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Mechanical stability of solids at negative pressures

Baidakov V G

Institute of Thermophysics of the Ural Branch of the Russian Academy of Sciences, Amundsen Street 107a, Ekaterinburg 620016, Russia

baidakov@itp.uran.ru

Using Gibbs ideas of the thermodynamic stability of homogeneous phases, we investigated the problem of the ultimate strength of an elastic (isotropic or crystalline) solid.
The elastic constants of a Lennard-Jones fcc crystal loaded with a hydrostatic pressure p have been calculated in molecular dynamics experiments. The bulk modulus K_T and the moduli of simple μ and tetragonal μ' shear have been determined. It is shown that in the case of homogeneous deformations the loss of stability of a solid at large negative pressures is connected with the bulk elasticity ($K_T = 0$) and at the positive and moderately negative pressures, with shear stresses ($\mu' = 0$). Inhomogeneous deformations in a solid, as distinct from homogeneous, are characterized by the coefficient of unilateral compression $\tilde{K}_T = K_T + (4/3)\mu$. It is shown that at large negative pressures this modulus has a finite value on the spinodal ($K_T = 0$). Thus, the boundary of essential instability of a solid here will be located beyond the spinodal. It is shown that the phase decay of a Lennard-Jones crystal at large stretches and temperatures higher than that of the endpoint of the melting line proceeds by way of formation and subsequent growth of liquid-phase nuclei, and lower, by way of initiation and growth of pores. It has been found that at the approach to the boundary of essential instability of a solid phase critical nuclei attain a shape close to spherical. Since at large negative pressures the shear moduli μ and μ' on the spinodal of a solid are positive, the work of formation of a critical nucleus here is different from zero, and it becomes possible to penetrate beyond the spinodal with retention of the activation mechanism of the phase decay. The work has been performed with a financial support of the Russian Science Foundation (project 14-19-00567).

Nitrogen phase transformation under quasi-isentropic compression up to 130 GPa

Ternovoi V Ya[@], Nikolaev D N, Kvitov S V and Pyalling A A

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] ternovoi@ficp.ac.ru

The most dense states in matter are generated dynamically by isentropic compression. This method is convenient to detect phase transitions and allows the full overview of states from zero to highest achievable pressure in one shot. The main increase of entropy in multiple shock compression process is caused by first shock in the investigated matter and depends on its intensity. The decrease of this shock and the absence of following strong shocks provides an opportunity to approach isentropic compression. A layered system consisting of polystyrene foam and steel layers was used to approach a compression path of nitrogen close to isentropic. Two ways to compress liquid nitrogen up to pressure of 110 and 130 GPa was elaborated. Optical self—emission and electrical conductivity measurements of compressed nitrogen were recorded in experiments. Modified Ross equation-of-state model for nitrogen was used in 1D hydrodynamic simulation of experiment. The comparison of the experimental records and results of hydrodynamic simulation made possible to evaluate density level at the moment of sharp increase of nitrogen conductivity. Density, pressure, temperature are following: 3.2 ± 0.1 g/cc, 75 GPa and 95 GPa, 3100 ± 200 K. These states are near the expected model boundary of liquid-liquid phase transition of molecular nitrogen–polymeric nitrogen

Deuterium compression isentrope: Analysis of temperature and electrical conductivity

Levashov P R[@], Minakov D V and Chentsov A V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] pasha@ihed.ras.ru

In this work we present our calculations of the compression isentrope of deuterium. We use a pseudopotential density-functional-theory (DFT) code VASP [1] with the plane-augmented-wave pseudopotential (with the lowest cut-off radius of 0.42 Å) and generalized-gradient-approximation exchange-correlation functional. The quantum molecular dynamics approach which is based upon the Born–Oppenheimer approximation is applied to calculate pressure and internal energy of dense deuterium plasma. The calculations were made in the range of temperatures 293–10^5 K and densities 1–3 g/cm^3. We use Zeldovich's approach [2] to restore the isentrope by two different ways and compare the results with experimental data and other theories [3]. We did not find a density jump registered experimentally [3]. However we found the sharp rise of electrical conductivity in the range of densities 1–2 g/cm^3. We also discuss temperature and structural transformation of deuterium along the isentrope.

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Thermodynamic and transport properties of CH_2 plasma in the two-temperature case

Knyazev D V[@] and Levashov P R

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] d.v.knyazev@yandex.ru

Thermodynamic, transport and optical properties of CH_2 plasma are important for the simulation of modern laser experiments [1]. We use the method based on the quantum molecular dynamics, density functional theory and the Kubo-Greenwood formula [2] to obtain necessary properties.

The properties of CH_2 plasma at $T_i = T_e = T$ were investigated in our previous work [3]. The most interesting results were obtaned for 5 kK $\leq T \leq$ 10 kK: rapid growth of static electrical conductivity $\sigma_{1_{\rm DC}}(T)$ and falling heat capacity $[C_v - C_{v\ i}^{\rm kin}](T)$ (i.e. concave $[E - E_i^{\rm kin}](T)$).

In this work we focus on CH_2 plasma in the two-temperature case $T_e \geq T_i$. The dependences of $\sigma_{1_{\rm DC}}$ and $[E - E_i^{\rm kin}]$ on T_i (5 kK $\leq T_i \leq$ 10 kK) at fixed $T_e = 10$ kK are close to the temperature dependences at $T_i = T_e = T$. Thus the dependences $\sigma_{1_{\rm DC}}(T)$ and $[E - E_i^{\rm kin}](T)$ at $T_i = T_e = T$ are mostly due to the influence of T_i.

The peaks at radial distribution functions (RDF) curves show the existence of chemical bonds at $T_i = T_e = 5$ kK. These bonds destroy rapidly as T_i grows and remain almost intact as T_e grows.

Thus, the growth of $\sigma_{1_{\rm DC}}$ and $[E - E_i^{\rm kin}]$ correlates with the decay of chemical bonds at 5 kK $\leq T_i \leq T_e \leq$ 10 kK.

This work was supported by the Ministry of Education and Science of the Russian Federation, grant No. 3.522.2014/K.

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Thermodynamic properties of LiD under compression with different pseudopotentials for lithium

Minakov D V[@] and Levashov P R

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] minakovd@ihed.ras.ru

In this work we analyze the contribution of the inner-shell electrons of Li and overlapping of pseudopotential cores to thermodynamic properties of ^{7}LiD under compression using density functional theory and quantum molecular dynamics (VASP [1]). At zero temperature there is no noticeable influence of 1s electrons of Li on pressure up to fivefold compression. However, shock compression reveals significant difference in pressure in calculations with 1 or 3 valence electrons for Li at pressures higher than 200 GPa. This fact can be explained by the weaker repulsion of Li ions with the frozen inner shell rather than by the excitation of the inner-shell electrons. We estimate conditions at which the one-electron pseudopotential is inapplicable in the unordered phase. Also we obtain new data on double shock compression of ^{7}LiD up to 1.2 TPa in good agreement with available experiments.

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Equation-of-state calculation for LiH and LiD based on quantum-statistical models

Kadatskiy M A[1,2,@] **and Khishchenko K V**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] makkad@yandex.ru

Various quantum-statistical cell models with the approximation of self-consistent field are widely used for development of equations of state. The application of these approximations is even more valid, the higher the temperature and the density of matter [1]. The separate and important issue is obtaining of the equation of state for the mixture. At that, the technique of determining the self-consistent potentials for a mixture of simple substances proposed by Orlov [2] is applied. For the cell-based models of matter, this technique allows to make equal the chemical potentials those are calculated separately for each component of the mixture.
In the work, calculated results are presented for Hugoniots of LiH and LiD based on quantum-statistical models with different electronic and ionic parts. Three models of electronic part are considered: the Thomas–Fermi, the Thomas–Fermi with quantum and exchange corrections and the Hartree–Fock–Slater models [1]. The influence of the thermal motion and the interaction of ions is taken into account in the framework of three models: the ideal gas, the one-component plasma and the charged hard spheres. Calculations are performed in the pressure range from 1 to 10^7 GPa. A comparison is done with results of other approaches and available data from shock-wave experiments [4] for LiH and LiD.

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Region of validity of the Thomas–Fermi model with quantum, exchange and shell corrections

Dyachkov S A[1,2,@], Levashov P R[1,2] and Minakov D V[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] serj.dyachkov@gmail.com

The equations of state (EoSs) under extreme conditions are of high importance for variety of applications in modern physics. The most promising approaches for construction of wide-range EoSs are based on the density functional theory (DFT) [1]. Nowadays, however, it is too difficult to perform such calculations at low densities and temperatures higher than several tens of eV. Hopefully, the region of validity of the well-known finite temperature Thomas–Fermi (FTTF) model [2] begins from tens of eV at normal densities and expands for higher temperatures and densities [3]. The properties of low density plasma can be also described well with the shell corrections [4]. To demonstrate linkage of models at temperatures between 10–100 eV we perform calculations of thermodynamic properties of metallic plasma within FTTF and DFT approaches at normal densities. For the low density plasma we compare FTTF with Saha model. Finally, the region of validity of FTTF with quantum, exchange and shell corrections is presented in wide range of parameters.

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Density of states on the surface of topological insulator with impurities based on the Thomas–Fermi theory

Akzyanov R S[1,2,@] **and Dyachkov S A**[1,2]

[1] All-Russia Research Institute of Automatics named after Dukhov, Luganskaya 9, Moscow 115304, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] akzyanov@vniia.ru

The Thomas-Fermi theory is widely used for calculation of equations of state for matter in extreme conditions [1]. The model is usually considered for the electrons in atomic spherical cell, but such approach is restricted for usage at normal conditions [2]. Approaches based on density functional theory provide complete information for the electronic structure of matter, but they are spatially restricted due to complexity and cannot be used for large systems. In the research [3] it was shown that the Thomas-Fermi theory can be applied for the description of density of states of quasiparticles in two-dimensional systems such as the surface of topological insulator or graphene. In resent experimental research [4] it was also shown that density of states is strongly influenced by the quasiparticle scattering on charged impurities. We investigate the applicability of the Thomas-Fermi approach with exchange and scattering corrections, perturbatively included in the density functional. Scattering on impurities calculated with the precise T-matrix method [5].

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Static polarizability in combined Thomas–Fermi model

Kyarov A Kh and Savintsev A P[@]

Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia

[@] pnr@kbsu.ru

The aim is to study the combined Thomas–Fermi model and based on its basis multipole static polarizability of atoms and, possibly, other particles of condensed matter, which are known potential distribution or electron density. The proposed model, first, used as a unperturbed electron density approximated Slater functions of the Hartree–Fock electronic distribution of atoms. Secondly, the choice of the perturbed electron density in the present model is based largely on the use of the results obtained in the framework of quantum-mechanical perturbation theory [1], and quantum electrodynamics [2]. Angered potential $\varphi(\vec{r})$ depends on unperturbed $\varphi_0(\vec{r})$ as follows [3]:

$$\varphi(\vec{r}) \propto \varphi_0(\vec{r}) exp\left(-\frac{\lambda}{\varphi_0(\vec{r})}\right).$$

However, this choice of the perturbing potential cannot be unambiguously regarded as going beyond the scope of the Thomas–Fermi method, as the minimization of the energy functional by Ritz method involves a fairly wide in the choice of trial functions, which of course does not exclude the need to physically clear rationale for this choice. The calculations of the static multipole polarizability for atoms with closed electron shells show good accuracy of the model. This work was supported in the framework of the base part of a government assignment issued by the RF Ministry of Education and Science to KBSU for years 2014–2016 (project 2014/54-2228).

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One-dimensional analytical solution of the Schrödinger equation using the periodic delta potential

Azeddine B

Laboratory of Semiconductor Device Physics of the Tahri Mohamed Bechar University, P.O.B. n°417, Bechar 08000, Algeria

bouziane60@mail.ru

Condensed matter physics is one of the most active and versatile branches of modern physics that have developed in the beginning of the discovery of quantum mechanics. It deals with problems concerning the properties of materials ranging from the fundamental needs of technological applications. Where the electron's moving in atoms and molecules don't obey to the classical Newton's motion equation. So, there are many good reasons to address the quantum mechanical theory beyond its historical significance. In this case, the movement of electrons is given by the Schrödinger equation which has two forms. In the first form, the time explicitly appears, and so describes how the wave function of a particle will evolve in time. The second form is the equation in which the time dependence has been removed and hence is known as the time independent Schrödinger equation and is found to describe, what the allowed energies are of the particle.

It is always challenging to solve the Schrödinger equation even the solution could be analytical or numerical. In this paper, we will describe how the time independent Schrödinger equation can be solved analytically using the approach of a particle moving in periodic delta potential [1,2] as a new way to find analytical solutions of this equation.

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The models for description of the Grüneisen coefficient

Belkheeva R K

Novosibirsk State University, Pirogova Street 2, Novosibirsk 630090, Russia

rumia@post.nsu.ru

To describe the material subjected to shock-wave action, the equation of state in the form of Mie–Grüneisen is used. If the shock wave is of low intensity, then the Grüneisen coefficient is assumed to be constant and equal to γ_0—the Grüneisen coefficient under standard conditions. If the shock wave is strong, then the formula

$$\gamma \approx \gamma_0 \left(\frac{\rho_0}{\rho}\right)^l, \tag{1}$$

is used.

Analysis of data given in the literature shows that with an increase in the intensity of shock-wave loads, the magnitude of the Grüneisen factor decreases. However, if the Grüneisen factor is described by (1) at large porosities and pressure, then it will increase in comparison with the normal value γ_0.

With the growth in loads, when the relative influence of thermal pressure increases in such a way that the matter density begins to decrease and turns out to be less than ρ_{T0}, the density dependence of the Grüneisen factor this paper proposes to describe by the equation

$$\gamma \approx \gamma_0 \left(\frac{\rho_0}{\rho}\right)^{-l}, \tag{2}$$

where the exponent l has the same value as in (1).

Besides relation (2) the Grüneisen coefficient logarithmic dependence of the density, and the Grüneisen coefficient dependence of the loading pressure are also considered.

A few-parameter equation of state of the condensed matter

Kraus E I[@] and Shabalin I I

Institute of Theoretical and Applied Mechanics of the Siberian Branch of the Russian Academy of Sciences, Institutskaya 4/1, Novosibirsk 630090, Russia

[@] kraus@itam.nsc.ru

Within the framework of the Mie–Grüneisen model, based on Molodets' version of the Grüneisen function [4], the present work describes the construction of the thermodynamic equation of state for the solid phase in the Debye approximation with the minimum number of parameters, where the "cold" pressures and energy are obtained in an analytical form from the generalized form of the Grüneisen function.

The expression obtained for the Grüneisen function allows one to find the equation for the zero isotherm and to analytically calculate the value for the "cold" components of pressure and internal energy and, hence, the thermodynamic expression of state for the solid phase with the thermal oscillations of the crystalline lattice are described by the Debye approximation.

To derive this equation, one has to know only six constants: specific volume V_0, volume expansion function β, isothermal K_t or adiabatic K_s modulus of volume compression, heat capacity at constant pressure c_P or at constant volume c_V, Debye temperature Θ, and electronic heat capacity c_{V_e}.

Two-dimensional problems of the high-velocity impact of the model reactor blocks of a nuclear powerplant onto the Earth surface were solved numerically on the basis of the elastoplastic model and with the use of the constructed equation of state [2].

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Thermodynamic parameters of heterogeneous materials under shock-wave loading in presentation of equilibrium model

Maevskii K K[@] and Kinelovskii S A

Lavrentyev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 15, Novosibirsk 630090, Russia

[@] konstantinm@hydro.nsc.ru

The results of numerical experiments on modeling of shock wave loading of solid and porous heterogeneous materials on the example of molybdenum and alloy including molybdenum in its composition as a component are presented. The model TEC (thermodynamic equilibrium components) is based on the assumption that all components of the material under shock-wave loading are in thermodynamic equilibrium. The equation of state of the Mie–Grüneisen type with allowance for the dependence of the Grüneisen coefficient on temperature is used for condensed phases [1, 2]. Model TEC allows us to describe thermodynamic parameters of molybdenum in a wide range of pressure and porosity in shock-wave compression and adiabatic unloading. Computational results are compared with the well-known experimental results obtained by different authors.The model parameters that allowed to reliably describe the thermodynamic parameters of pure molybdenum under shock-wave loading, were used for modelling molybdenum alloys with materials such as titanium, rhenium, uranium. It is shown that the proposed model can adequately describe the shock-wave loading of the considered alloys. The model permits the shock-wave loading of alloys with molybdenum in their composition to be described reliably solely by using species parameters.

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Hydrostatic and shock-wave compression of a molecular crystal

Degtjarjov A A[1,@], Smirnov E B[1], Kostitsyn O V[1], Stankevich A V[1], Muzyrya A K[1], Badretdinova L Kh[2], Ten K A[3], Pruuel E R[3] and Kashkarov A O[3]

[1] Federal State Unitary Enterprise "Russian Federal Nuclear Center—Academician Zababakhin All-Russian Research Institute of Technical Physics", Vasilieva 13, Snezhinsk, Chelyabinsk Region 456770, Russia
[2] Kazan National Research Technological University, Karl Marx Street 68, Kazan, Tatarstan 420015, Russia
[3] Lavrentyev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 15, Novosibirsk 630090, Russia

[@] a.a.degtjarjov@gmail.com

Thermodynamics of high-molecular organic compounds and especially metastable chemical compounds, both being energy-saturated materials, turns out to be a poorly studied area despite its practical importance. Theoretical determination of relationships characterizing behavior of solid energy-saturated materials runs into difficulties as they belong to molecular crystals and molecules constituting a crystal have great many internal degrees of freedom. The paper analyzes experimental data on the hydrostatic and shock-wave compression of the energy-saturated material. The Mie–Grüneisen–Debye semi-empirical equation of state based on the Helmholtz potential is used to describe thermodynamic properties of metastable molecular crystals without phase transitions taken into account. The equation of state describes experimental data on isothermal compression of a molecular crystal with the above data given by the powder diffraction analysis using diamond anvils. An expression for the Hugoniot curve satisfactorily describes the data on shock compression of the material having different initial porosity. The proposed equation of state is expected to give higher-accuracy description of thermodynamic properties of the energy-saturated material in numerical simulation of shock-wave and detonation processes.

Diamond high-temperature destruction mechanism

Basharin A Yu[@], Dozhdikov V S and Levashov P R

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] abasharin@bk.ru

To increase resistance of diamond to high-temperature heating is an important issue for its use as diamond anvils, laser mirrors and windows. To solve this problem, the mechanism of high-temperature destruction of diamond should be determined. The mechanism presented below were obtained from experimental observations and MD simulation. To eliminate the influence of the chemical interaction, diamond heating was produced from contact of graphite melt. Metallographic section study show that under a solidified drop subsurface bubbles and the crushed diamond, bonded by non-diamond carbon exists as initial and finished stages of destruction. Wedge-shaped inclusions in the diamond particles contained martensitic graphite. On the specifics of graphite structure it was found that diamond is under pressure 5–10 GPa. Structure similar to "crushed glass", which are specific for fracture failure there was found. The amorphous carbon, containing discontinuities indicates the melting of the diamond and cavitation under extension of liquid. According to MD, diamond does not melt when stretched to less than 60 GPa. It cannot be obtained in experiment and, therefore, only compressed diamond melts. The following mechanism has been proposed. Diamond graphitization in local regions (bubbles) leads to increase in carbon volume and pressure on a diamond appears. Due to decrease in thermal conductivity the diamond is superheated and highly compressed diamond is melted. The melting causes relaxation of mechanical stresses in unfused diamond and "ground glass" structure occurs. Interference or reflection of compression waves from boundaries of fluid leads to negative stress and disintegration of liquid as a result of nucleation, growth and merging of discontinuities. Proposed high-temperature mechanism is significantly different from low-temperature mechanism of brittle fracture of dielectrics.

Thermodynamic stability of detonation nanodiamonds

Efremov V P[1] and Zakatilova E I[1,2,@]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

[@] ei.zakatilova@mail.ru

Utilisation ammunitions with high explosives and the obtaining nanodiamond as result detonation synthesis have given new motivation for search areas their application. Nanodiamonds have next attractive properties: high density (3.51 g/cc), ultra high thermal conductivity and high dielectric properties. Use as fillers of nanodiamonds will allow to regulate heat conductivity, density, a thermal capacity and dielectric properties. In this work the stability of nanodiamond powder have been researched by method synchronous thermal analysis. Experiments have been conducted at atmospheric pressure of argon. Nanodiamond powder were heated in the closed crucible (Al_2O_3) in a temperature range of 30–1500 °C. After heat treatment, the samples have been researched by x-ray diffraction and electron microscopy. As a result of this work it have been found that temperature stability of part of nanodiamonds exceeds 1500 °C. This is rather unusual results expiring noun literature data.

Liquid carbon properties and structure: Modeling by quantum and classical molecular dynamics

Dozhdikov V S[@], Basharin A Yu, Levashov P R and Minakov D V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vdozh@mail.ru

Our previous experimental work was devoted to phase transitions in liquid carbon (LC) under conditions of intense heat exchange with a cold diamond substrate. LC quenching in this experiment led to the formation of a new carbon phase with amorphous structure. In this amorphous state carbyne–allotropic modification with sp atoms—is detected. Investigation of the structure and properties of the amorphous carbon will allow us defining areas of its possible application. This task cannot be performed experimentally and require molecular dynamics (MD). The quenching of LC by the classical MD showed the presence of a certain amount of sp atoms in the amorphous structure. But the amount of the sp atoms is dependent on classic potential type. Probably this is due to the complexity of the LC simulation with classical potentials. In this work we are trying to determine which of classical potentials describes LC most adequately. This will be achieved by comparing the density and structure of LC, received with various classical potentials with first-principle calculations. We used quantum MD implemented in the VASP package. For classical MD calculations the software LAMMPS and 4 classical potentials were used. We calculated the density and distribution of chemical bonds in LC at temperature 6000 K and pressures 1.2–17 GPa. It was found that for the description of LC one needs to use different classical potentials for different pressure ranges. In the next stage we plan to study amorphous carbon properties in more detail. This work was supported by RFBR (grants 16-08-01295, 13-08-01098).

Fluid–fluid–solid triple point on melting lines at high temperatures

Norman G E[@] and Saitov I M

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] genri.norman@gmail.com

Two predictions are formulated by Norman and Starostin in1968. The first one is "plasma phase transition". The second prediction is a fluid–fluid–solid triple point on the melting line at high temperatures. However they do not discuss the nature of the fluid–fluid transition. Such a triple point is observed experimentally first by Brazhkin et al for selenium in 1989. They point to the semiconductor–metal nature of the transition.

An analysis is presented of the subsequent experimental works where fluid-fluid phase transitions are observed at high temperatures with triple points on the melting curve. Data are given for different substances as Se, P, Sn, Bi, Te, S, Fe, Ce and some others. Viscosity drops point to the structural character of the transition, whereas conductivity jumps remind of both semiconductor–metal and plasma nature. The slope of the phase equilibrium dependencies of pressure on temperature and the consequent change of the specific volume, which follows from the Clapeyron–Clausius equation, are discussed. $P(V,T)$ surfaces are presented and discussed for the phase transitions considered in the vicinity of the triple points. The cases of abnormal $P(T)$ dependencies on lines of phase equilibrium are in the focus of discussion. In particular, a $P(V,T)$ surface is presented when both fluid–fluid and melting $P(T)$ lines are abnormal. Particular attention is paid to warm dense hydrogen and deuterium, where remarkable contradictions exist between data of different authors. The possible connection of the $P(V,T)$ surface peculiarities with the experimental data uncertainties is outlined.

The work is supported by the Russian Science Foundation (grant No. 14-50-00124).

Two-scale model of aluminum melting and its application for problem of electron beam irradiation

Krasnikov V S[@] and Mayer A E

Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia

[@] vas.krasnikov@gmail.com

Molecular-dynamics (MD) simulations of the non-equilibrium melting of aluminum are performed both with and without accounting of the electronic subsystem. A continuum model of melting is purposed basing on the obtained MD results, in which the current phase state is described in terms of fields of concentration and size of melting sites. Growth equation for melting areas is derived from the heat fluxes analysis. Nucleation equation for melting sites is formulated basing on the thermofluctuational approach. The method of determination of the model coefficients with using the MD simulation results is purposed. The continuum model is applied to the problem of the non-equilibrium melting of aluminum within the energy absorption area of the high-current electron beam.

Dynamics of phonon spectrum and anomaly of the curve of melting of sodium at pressures 0–60 GPa

Chingina E A[@] and Volkov N B

Institute of Electrophysics of the Ural Branch of the Russian Academy of Sciences, Amundsen 106, Ekaterinburg 620016, Russia

[@] zhenya@iep.uran.ru

Modern methods of research of structure of substances with high pressures [1], allowed to find not simple behavior of simple metals. For example, it is the abnormal character of curves of melting $T_m(P)$.

We used the software package of LmtART-7 [2] for finding of phonon and electron spectrum, and also—for finding of a total energy of interaction of electrons with sodium nuclei. Interaction potential on the basis of qualitative methods of the theory of a chemical bond is offered. This potential depends on characteristics of a complex lattice. It also depends on number of atoms in an elementary cell and contains small number of free parameters. We use the calculated values of a total energy for finding of these parameters.

For the description of liquid metal at high pressures the model according to which liquid consists of clusters with a quasicrystal order and defective intercluster boundary is used. Expressions for free energy and Gibbs' potential are presented. The curve of melting and jumps of volume and entropy of Na depending on pressure from equality of potentials of Gibbs on interphase boundary are obtained. Comparison with experiment is made.

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Recent advances in laser-pulse melting of graphite

Vervikishko P S[@] and Sheindlin M A

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] pvervikishko@gmail.com

Melting temperature of graphite and nature of liquid carbon remains a subject of permanent discussions in the literature for many decades. The main reason of this inconsistency is the extremely high melting temperature of graphite making it the most refractory material. The important aspect of this work is to study the nature of the cusp on the thermogram in the melting region. Unlike to other materials, the heating rate in liquid is higher than in solid state. Understanding this phenomenon may help to investigate the changes of thermal conductivity between solid carbon and liquid in wide pressure range. The melting thermogram was obtained for isotropic graphite at pressures 0.5–6 kbar.

Another important aspect of this study is crystallization of liquid carbon. Visualization of liquid phase was made by high-speed camera. To reduce the influence of thermal radiation, the interference filter was mounted in the camera optics and the sample surface was lighted by diode laser with optical power 100 W. Analysis of solidified liquid carbon and vapor condensate was made by scanning electron microscope. At high pressures were observed the vapor-liquid-solid mechanism of crystallization. In some experiments, we obtain the analog of nanowhiskers. Solidified liquid carbon whiskers differ from classical crystals because of different velocities of growth but they have the analogous proportions of length and diameter and the analogous mechanism of growth.

The drops of recrystallized carbon were obtained in different medium pressures, heating rate and cooling rate. At the cooling stage, laser power is not zero, the sample heated by 100–300 W for 10–15 ms to decrease the cooling rate. It helps us to realize slow crystallization mode.

The melting curve of graphite

Rakhel A D

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

rakhel@oivtran.ru

Direct measurements of thermophysical properties of graphite and liquid carbon have been made recently in our laboratory [1]. Those results were used here to estimate location and the slope of the melting curve of graphite in the pressure-temperature plane. It is shown that the slope of the melting curve based on the results [1] differs essentially from those of other literature experimental data. Reasons for the discrepancy are discussed. An attempt was made to determine location of the maximum in the dependence of the melting temperature on pressure because this feature may be related to a first order liquid I—liquid II phase transition in liquid carbon.

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On the kinetics of graphite melting: A molecular modeling approach

Orekhov N D[1,2,@] and Stegailov V V[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] nikita.orekhov@gmail.com

Experimental data on graphite melting temperature T_m still remain controversial despite the long history of investigation [1]. The results of several experimental works cover the wide span from 3800 to 5000 K that is an essentially larger uncertainty than the errors of individual experiments. Despite sophisticated theoretical and modeling efforts this question has not been resolved yet. In this talk, based on molecular dynamics (MD) and the accurate interatomic potential for carbon, we report our new results [2–4] on the kinetics of graphite melting (aspects of defect formation, single graphene layer melting and rates of liquid nucleation). We determine by thermodynamic integration the value of $T_m \approx 3650$ K. Our MD results show an unexpectedly weak kinetics of the melting front propagation in graphite that is several orders slower than that in metals. We demonstrate that at heating rates higher than 10^5-10^6 K/s graphite can be superheated 500-1000 K above Tm at the microsecond timescale. It allows us to explain the long-standing discrepancy in the experimental data on T_m. Besides, we discuss the pressure dependence of the T_m and the influence of the MD interatomic model choice.

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Melting of fcc and bcc lattices for the systems with various isotropic pair potentials

Vaulina O S[1,2,@] **and Koss X G**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] olga.vaulina@bk.ru

The melting of face-centered cubic (fcc) and body-centered cubic (bcc) crystal lattices was studied analytically and numerically for the systems with various isotropic interaction potentials, namely for the systems with inverse-power-law and Yukawa interaction potentials. The comparison of the obtained results with existing data is presented.
The new approximation for the determination of equilibrium melting curves of the systems is proposed. The suggested approximation takes into account the influence of nonlinearity (anharmonicity) of the pair interaction forces and allows to correctly predict the conditions of the melting of the systems with various isotropic interaction potentials, unlike the known empirical and half-empirical approximations. Characteristic frequencies and energies of crystal lattices were estimated within the framework of the nearest-neighbour approximation, and the amplitudes of the oscillations of particles in the nodes of the lattice were evaluated with the help of Lindemann parameter on the melting lines of the systems under study.
Notice that the scope of proposed approach is not limited by considered potentials. The presented model may be easily adapted for a wide range of systems with isotropic repulsive potentials and may be useful for estimations of solid-liquid phase curves and fcc–bcc–liquid triple point.
This work was supported by the Russian Foundation for Basic Research (grant No. 16-08-00594), by the Ministry of Education and Science of the Russian Federation and by the Presidium of the Russian Academy of Sciences.

Equation of state based on linear model and phenomenological theory of the critical point

Rykov V A[@] and Rykov S V

Saint-Petersburg State University of Information Technologies, Mechahics and Optics, Kronvergskiy 49, Saint-Petersburg 197101, Russia

[@] togg1@yandex.ru

The report describes the method of constructing scale equation of state in variables density and temperature. This method is based on the Benedek hypothesis. According to this hypothesis, the behavior of the isochoric heat capacity C_V and the coefficient of isothermal compressibility K_T at the critical and near-critical isochore are described by the same power laws:

$$X = A\left|\frac{T - T_X(\rho)}{T_c}\right|^{-\chi}, \tag{1}$$

where $X = C_v$, $\chi = \alpha$ and $X = K_T$, $\chi = \gamma$. It is shown that from Schofield–Litster–Ho linear model (LM) follows that the singular component of the chemical potential has the form

$$\Delta\mu = \varphi_0 \Delta\rho (C_v/T)^{-\gamma/\alpha} + \varphi_2 (\Delta\rho)^3 (C_v/T)^{(2\beta-\gamma)/\alpha}. \tag{2}$$

On the other hand, from phenomenological Migdal theory of the critical point, it follows that $\Delta\mu$ can be represented in the form

$$\Delta\mu = \varphi_1 K_T^{-1} + \varphi_3 K_T^{(2\beta-\gamma)/\gamma}. \tag{3}$$

On the basis (1)–(3), scale function of the chemical potential $h(x)$ in variable density and temperature is calculated as

$$h(x) = \sum A_i (x + x_i)^{\gamma} + \sum B_i (x + x_i)^{\gamma - 2\beta}. \tag{4}$$

It is shown that the function (4) has only two fitting parameter, and the relative error $\delta h = (h_l(x) - h(x))/h_l(x)$ does not exceed 1% (h_l—LM scale function).

Fundamental equation of state of perfluoropropane

Kudryavtseva I V, Rykov V A and Rykov S V[@]

Saint-Petersburg State University of Information Technologies, Mechahics and Optics, Kronvergskiy 49, Saint-Petersburg 197101, Russia

[@] togg1@yandex.ru

In the report describes the method of constructing the fundamental equation of state (EOS), based on a large-scale representation of the hypothesis in the form of equation:

$$\Delta S X^{(1-\alpha)/\chi} = \varphi_0 + \varphi_2 m^2, \quad m = \Delta\rho X^{\beta/\chi}. \tag{1}$$

Here $\Delta S = (\rho_c T_c/p_c)\left[S(\rho,T) - S_0(T)\right]/f(\omega)$; S—the entropy; $f(\omega)$—the crossover function; $\Delta\rho = \omega - 1$; $\omega = \rho/\rho_c$; α, β, χ—the critical indices; X—thermodynamic function having a singularity at the critical point, which is characterized by the critical index (for example, if $X = K_T$ $\chi = \gamma$). The fundamental equation of state, which follows from (1) has the form

$$\frac{\rho}{p_c}F(\rho,T) = \frac{\rho}{p_c}F_{\text{reg}}(\rho,T) + f(\omega)\,|\Delta\rho|^{\delta+1}a(x), \tag{2}$$

where $F(\rho,T)$—the Helmholtz free energy; $a(x)$—the scale function. If in the equation (2) put $f(\omega) = 0$, then equation (2) coincides with the equation of state in virial form. On the basis of fundamental equation (2), equation of state of perfluoropropene is designed, which in regular field of thermodynamic surface satisfies all the requirements of the equations of state in virial form. The equation of state (2) satisfies the scale hypothesis in the vicinity of the critical point and with a small error reports experimental data of equilibrium properties of perfluoropropene. For example, the maximum deviation of the density calculated by equation (2) from the experimental data is 0.02% in a dense fluid and 6% in the vicinity of the critical point. At the same time, the size of $\delta\rho_{\max}$ is 0.3% in a dense fluid and 35% in the vicinity of the critical point for the fundamental equation of state by Lemmon and Span (2006).

The fundamental equation of state for R32 that meets the requirements of the scale theory

Rykov S V[@], Kudryavtsev D A and Rykov V A

Saint-Petersburg State University of Information Technologies, Mechahics and Optics, Kronvergskiy 49, Saint-Petersburg 197101, Russia

[@] togg1@yandex.ru

The authors reviewed the method of constructing the fundamental equation of state based on the representation of scale hypothesis in the form of equation

$$\Delta S X^{(1-\alpha)/\chi} = \varphi_0 + \varphi_1 m^2 + \varphi_3 X^{-\Delta/\chi} + \varphi_4 X^{-\Delta/\chi} m^2, \quad (1)$$

where $m = \Delta\rho X^{\beta/\chi}$, $\Delta S = (\rho_c T_c/p_c)\left[S(\rho,T) - S_0(T)\right]/f(\omega)$; S—the entropy; $f(\omega)$—the crossover function; $\Delta\rho = \omega - 1$; $\omega = \rho/\rho_c$; α, β, χ and Δ—the critical indexes; X–the thermodynamic function, having a singularity at the critical point, which is characterized by the critical index (for example, if $X = K_T$, then $\chi = \gamma$). The fundamental equation of state, which follows from (1) has the form

$$F(\rho,T) = F_{\text{reg}}(\rho,T) + f(\omega)\,|\Delta\rho|^{\delta+1}\left[a_0(x) + u|\Delta\rho|^{\Delta/\beta} a_1(x)\right], \quad (2)$$

where $F(\rho,T)$—the Helmholtz free energy; $a_i(x)$ $(i = 0,\ 1)$—the scale functions of F $(\Delta_0 = 0,\ \Delta_1 = \Delta)$. The fundamental equation of state (2) with scale functions approved by the example of the thermodynamic description of the surface of R32. We calculated the table of equilibrium properties of R32 in the state parameters: temperature from 136.34 to 420 K and pressure up to 40 MPa. Also, we calculated the detailed thermodynamic tables for the general vicinity of the critical point. Calculations showed that the accuracy of calculation of the equilibrium properties in the regular part of the thermodynamic surface by equation does not yield to the proposed equation (Tilner–Roth 1997), and in the critical region—Kiselev crossover equation.

The equation of state of argon taken into account the asymmetry of the liquid relative to the critical isochore

Kudryavtseva I V[@], Rykov S V and Rykov V A

Saint-Petersburg State University of Information Technologies, Mechahics and Optics, Kronvergskiy 49, Saint-Petersburg 197101, Russia

[@] togg1@yandex.ru

On the basis of the proposed model of scale hypothesis, an expression was obtained for the singular part of the entropy S:

$$\Delta S\left(\rho,T\right)=\sum_{n=1}^{3}\sum_{i=0}^{3}X_n^{(\alpha-1-\Delta_i)/\chi_n}\left[\varphi_{n-1,i}+\varphi_{n,i}m_n+\varphi_{n+1,i}m_n^2\right], \tag{1}$$

$$m_n=\tau_p^{\beta}X_n^{\beta/\chi_n}. \tag{2}$$

There $\tau_p=\tau/\tilde{x}$; $\tilde{x}$—the generalized scaled variable [1]; $\tau=T/T_c-1$; X—the thermodynamic function, having a singularity at the critical point, which is characterized by the critical index (for example, if $X=C_V$, then $\chi=\alpha$). On the basis of (1), a scale function of the free energy $a_n\left(\tilde{x}\right)$ is calculated. The fundamental equation of state of an argon is developed, which is based on functions $a_n\left(\tilde{x}\right)$. This equation allows taking into account the asymmetry of the liquid relative to the critical isochore. We have calculated the table of equilibrium properties of argon in a wide range of state parameters: density to $3.35\rho_c$, the temperature from the triple point to 1000 K. It is shown that the error δC_V in the description of experimental data C_V from Voronel *et al* (1965) and Anisimov *et al* (1975, 1978) in the vicinity of the critical point does not exceed 10%. While the δC_V calculated by the crossover equation of state [2] from Voronel *et al* (1965) exceeds 100%.

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A comparative study of scaling models for the densities on the coexistence curve

Ustyuzhanin E E[@], Vorobev V S and Shishakov V V

National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

[@] evgust@gmail.com

Some group of models $F = F(t, D, C)$ is investigated in the report. These models are connected with thermodynamic properties, $F = (\rho_l, \rho_g, f_s, f_d \ldots)$, including the densities, ρ_l, ρ_g, related to the coexistence curve (CC), the order parameter, f_s, and the coexistence curve diameter, f_d. $F(t, D, C)$ models include critical characteristics, $D = (\alpha, \beta, T_c \ldots)$, a relative temperature, t, coefficients, C, and follow to the scaling theory of critical phenomena. These models of properties are represented by equations of Wegner (1985), Anisimov *et al* (2006), Rabinovich and Sheludiak (1995), Shimanskaya *et al* (1996), Bazaev, Abdulagatov *et al* (2007). One more model $F(t, D, C)$ is named as a combined model (CM) and proposed to express properties $F = (\rho_l, \rho_g, f_s, f_d)$ in this work. It combines scaling, F_s, and regular, F_r, parts. Its description is given in [1] and [2]. CM model, $f_d = F(t, D, C)$, uses a leading component that includes a characteristic $D = 2\beta$. This model is related to modern equations of ST. CM models of $F = (\rho_l, \rho_g, f_s, f_d)$ are adopted to experimental (ρ_l, ρ_g, t) data of several substances and compared with equations mentioned earlier. For example some numerical results are got for CM models of SF_6 including CC diameter $f_d = F(t, D, C)$; elaborated models are compared with equations of Anisimov *et al* (2006), Wagner [3] and others.

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Critical factor of compressibility: The characteristic of the equation of state and a physical parameter

Petrik G G

Institute for Geothermal Research of the Daghestan Scientific Center of the Russian Academy of Sciences, Shamil 39a, Makhachkala, Daghestan 367030, Russia

galina_petrik@mail.ru

The impossibility of exact calculation of thermodynamic properties on the basis of molecular information compels to pass to model representations at two specified levels. Thus we consider as important to be based on ideas of system approach according to which any change in a form of the equation of state (EOS) follows and has to be explained with changes in molecular model. Such view convinces at least that the approach of authors of many low-parametrical van-der-Waals type EOS is incorrect because changing the EOS form and increasing number of parameters they keep molecular notions of van-der-Waals (sense of two EOS parameters—a and b). This fact forces the authors to design the EOS so that the critical factor of compressibility (CFC) was more than the physical characteristic. It is known that the "experimental" values of CFC belong to a narrow interval 0.30–0.25. We did not meet explanations for this fact in literature. However, the results obtained by us when realizing the opportunities of the simplest molecular models–the interacting point centers and spherical shells—and the new EOS constructed on their basis allow to answer many questions including concerning observed values of CFC. Recently it was succeeded to build hierarchy of the different levels control parameters in the form of analytical formulas connected with each other. Giving an interval of 0–0.5 for degree of overlapping "atoms" in "molecule" and changing quantity of the atoms, which determines the greatest linear extent of the object—2, 3, 4, . . . —having applied calculation formulas, we not simply have obtained as a result the observed interval of CFC values, but also have revealed the structure of this interval.

Practicing the two-level molecular-statistical method for describing the structure and thermodynamic properties of molecular medium in different aggregative states

Narkevich I I[@] and Farafontova E V

Belarusian State Technological University, Sverdlova Street 13a, Minsk 220006, Belarus

[@] inarkevich@mail.ru

Using the two-level molecular-statistical approach, a single state equation for the crystal, liquid and gas have been obtained:

$$p = -\frac{\theta}{\omega}\ln\left(1-\frac{\omega}{\upsilon}\right) - \frac{A\omega}{2\upsilon^2} - \frac{\omega^2}{2\upsilon^3}\left(\frac{\partial A}{\partial n}\right)_{\theta,\omega}. \qquad (1)$$

Here $\theta = kT$, $\upsilon = V/N$ is a molecular volume, ω is a microcell volume, $n = N/M$ is a concentration of molecules in the volume V of system, which is divided into M microcells, $M = V/\omega$ is the number of microcells, a volume of which is ω, A is an energy-entropy parameter of model, calculated by solving the integral equation for the potentials of average forces, which is an element of Rott's method of conditional distributions. The free energy of the system in the F_{11}-approximation of conditional distributions corresponding to equation (1) has the form

$$F = U - TS = \theta\frac{N}{n}\left(n\ln n + (1-n)\ln(1-n)\right) - N\frac{An}{2}. \qquad (2)$$

As a result, the free energy and the pressure in crystalline and liquid states of the system for three temperatures, which are located between the temperature of the triple point and temperature of the critical point, were calculated.

Attachment and accommodation at cluster growth in metal vapor

Lenev D Y[1,2,@] **and Norman G E**[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] lenevdy@mail.ru

Attachment and thermal accommodation coefficients are calculated, which are necessary to describe condensation kinetics in supercooled vapors. Molecular dynamics (MD) method is applied as in [1, 2]. Smaller clusters and other temperatures are studied in [1]. In [2], thermal accommodation coefficient for a flat surface and only one temperature is calculated

A system of a spherical nucleus of liquid phase and a single incident atom is studied. Finnis-Sinclair potential is used for describing interactions between atoms of the cluster. The incident atom interacts with cluster atoms by the Lennard-Jones potential. Attachment coefficient is a fraction of MD runs, which results in sticking of the incident atom to the cluster. Thermal accommodation coefficient is equal to the ratio of the incident atom kinetic energy loss to the difference between cluster and incident atom temperatures. 500 of similar MD runs are repeated with velocities of the incident atom distributed according to Maxwell for averaging. The coefficients are obtained for 7 temperatures from 1200 to 4500K and cluster sizes of 27, 113 and 339 atoms; incident atom temperature equals 300K. Dependencies of the attachment coefficients on the impact parameter of the incident atom are calculated. Thermal accommodation coefficients obtained are compared with [2] and experiment [3].

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Conductivity of metal vapors in vicinity of critical point

Khomkin A L and Shumikhin A S[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] shum_ac@mail.ru

A few years ago we suggested a hypothesis that cohesive coupling of atoms remains up to some small, but gas vicinity of the vapor-liquid critical point and therefore the value of cohesive energy can use for thermodynamic calculations of parameters of the critical point. Critical point parameters and binodal were calculated practically for all metals of the periodic table [1] with use of the Helmholtz free energy, based on this hypothesis. In this study the problem for calculation of conductivity of metals in vicinity of critical point within uniform physical model is considered (in a complex). Conductivity is experimentally measured only for alkaline metals and mercury [2]. Available calculations of conductivity are made for alkali metal vapors and mercury for known composition of vapors along binodal, i.e electron density and conductivity are calculated independently. Being important value in itself, conductivity in a critical point supplements a traditional set of critical parameters and distinguishes vapor-liquid transition in vapors of metals from traditional transitions. The conductivity at the critical point can be called the fourth critical parameter. For calculation of conductivity it is necessary to know the concentration of conductivity electrons. Some ways of its calculation are considered. Conductivity is calculated using a Rigel-Ioffe formula. Our calculations are qualitative agreed with experimental data for Cs and Rb. For other metals conductivity in critical point is calculated in first. This study is performed with financial support of the Program of basic researches of Presidium of the Russian Academy of Sciences "Substance at the high energy density".

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Pseudocritical point in anomalous phase diagrams of simple plasma models

Chigvintsev A Yu[1,@], Iosilevskiy I L[1] and Noginova L Yu[2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
[2] Russian State Agrarian University—Timiryazev Moscow Agricultural Academy, Timiryazevskaya 49, Moscow 127550, Russia

[@] alex012008@gmail.com

Anomalous phase diagrams in subclass of simplified (non-associative [1]) Coulomb models are under discussion. The common feature of this subclass is absence on definition of individual correlations for charges of opposite sign. It is e.g. modified OCP of ions on *uniformly compressible* background of ideal fermi-gas of electrons {OCP(∼)}, or a superposition of two non-ideal OCP(∼) models of ions and electrons etc. In contrast to the ordinary OCP model on *non-compressible* (rigid) background {OCP(#)} two new phase transitions with upper critical point, boiling and sublimation, appear in OCP(∼) phase diagram [1, 2] in addition to the well-known Wigner crystallization. The point is that the topology of phase diagram in OCP(∼) becomes anomalous at high enough value of ionic charge number Z [2, 3]. Namely, the only one *unified crystal-fluid* phase transition *without critical point* exists as continuous superposition of melting and sublimation in OCP(∼) at the interval $(Z_1 < Z < Z_2)$. The most remarkable is appearance of *pseudocritical points* at both boundary values $Z = Z_1 \approx 35.5$ and $Z = Z_2 \approx 40.0$. It should be stressed that critical isotherm is exactly *cubic* in both these pseudocritical points.

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Effect of high pressure on the crystal structure of chalcogenides based on layered semiconductors

Melnikova N V[@] and Volkova Ya Yu

Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

[@] nvm.melnikova@gmail.com

Layered semiconductors A^3B^6 (InSe, InS, GaSe, etc) and chalcogenides based on them such as $CuInCh_2$, $(InCh)_{1-x}(CuAsCh_2)_x$, Ch—chalcogenides, demonstrate a combination of interesting electrical, optical and other physical properties, and undergo baric and temperature phase transitions. Some of them demonstrate negative magnetoresistance (NMR) under high pressure at room temperatures. The causes of NMR in semiconductors at high pressures have not been studied in detail. The aim is to investigate influence of high pressure on the crystal structure of $(InSe)_{0.5}(CuAsSe_2)_{0.5}$, exhibiting NMR [2], at pressures up to 60 GPa. Crystal structure was studied by high pressure Raman scattering spectroscopy and synchrotron x-ray diffraction technologies. High pressure was applied to the samples using helium pressure medium in a diamond anvil cells. With pressure increasing two structural transitions were observed: from chalcopyrite structure to a cubic NaCl-type in the range 8–10 GPa and from NaCl-type to the orthorhombic structure in the range 32–38 GPa, analogously to transitions in tetragonal $CuInSe_2$ [2]. The observed noticeable changes in a behavior of magnetoresistance and other electrical properties in these pressure ranges are caused by structural transitions and due to a change of electron structure.

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Study of temperature dependences of electric properties of amorphous silver chalcogenides containing carbon nanotubes

Kurochka K V[@] and Melnikova N V

Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

[@] kirill.k.v@yandex.ru

This work is devoted to the study of the temperature dependence of electrical properties of $AgGe_{1+x}As_{1-x}(S+CNT)_3$ ($x = 0.4$, 0.5, 0.6) materials with the addition of carbon nanotubes at temperatures range from 10 to 300 K. The synthesis of materials and their properties at room temperature described in detail in [1, 2].

Electric properties of the materials in the temperature range 10–300 K was studied on ac in the frequency range where the sample contacts with electrodes do not affect on measurement of samples properties.

Temperature ranges in which there is a significant change in the behavior of all investigated electric properties (real and imaginary parts of the impedance, conductivity, permittivity) for all materials were determined. On the temperature dependence of the real parts of impedance maxima are observed for all three materials. Similar behavior of $\mathrm{Re}Z$ was observed in materials from the system Cu-Ag-Ge-As-Se [3], maxima on the curve of $\mathrm{Re}Z(T)$ located in the near of the temperature corresponding to the beginning of a significant ion transport.

The study was supported by the Russian Foundation for Basic Research, project 16-32-00350 mol_a and by the Foundation for Assistance to Small Innovative Enterprises in Science and Technology.

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Study of electrical properties of multicomponent silver and copper chalcogenide glasses at temperatures range 300–400 K

Zaikova V E[@], Melnikova N V, Kurochka K V and Kheifets O L

Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

[@] vasilisazaykova@gmail.com

This work is deal with the temperature dependence of electrical properties of chalcogenide glasses $Cu_{1-x}Ag_xGeAsSe_3$, $0.9 \geq x \geq 0.7$ at temperatures range from 300 to 400 K. These materials are well known as mixed (ionic–electronic) conductors, with many interesting properties both from theoretical and practical point of view [1–4].

Temperature dependences of electric properties of the investigated materials were studied on dc and ac (1 Hz–32 MHz). Time dependences of conductivity and frequency dependences of impedance and complex conductivity were measured at all investigated temperatures.

With the temperature increasing the rise of the conductivity as exponential function was observed both on dc and ac, and the type of hodographs (semicircle at high-frequency part) are retained. The activation energy and the relaxation time of carries for all studied materials were estimated.

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Influence of external effects on the dielectric properties of $Ln_{2-x}Sr_xNi_{1-y}M_yO_4$

Yakovleva E A[1,@], Melnikova N V[1], Chupakhina T I[2] and Kadyrova N I[2]

[1] Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia
[2] Institute of Solid State Chemistry of the Ural Branch of the Russian Academy of Sciences, Pervomaiskaya Street 91, Ekaterinburg 620219, Russia

[@] katrina.yakovleva@inbox.ru

The main trend in the development of microelectronics is the miniaturization and increase performance of various devices. Compounds of the system $Ln_{2-x}Sr_xNi_{1-y}M_yO_4$ (M = Cu, Co, Fe, Ni; Ln = La, Nd, Sr, Ca) are promising for electrochemical structural elements and microelectronic technologes [1, 2]. The study of these materials offers the prospects for the miniaturization of capacitive elements.The purpose of this study is to identify the impact of external factors—the concentration ($0.2 < x$, $y < 0.8$), temperature (10–600 K), the frequency of the external electric field (10 μHz–32 MHz), pressure (up to 30 GPa)—on the electrical properties of materials $Ln_{2-x}Sr_xNi_{1-y}M_yO_4$, synthesized by sol-gel method (SAF) and the further use of thermobaric treatment for some samples, in terms of fixed and variable electric field, establishing the presence of high dielectric constant of these compounds. Analysis of the connection between the structural parameters of materials with their dielectric properties revealed that the dielectric constant increases as the deviation from the ideal structure.

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Martensitic transformation and nanoscale aspects in shape memory alloys

Adiguzel O

Firat University, Elazig 23169, Turkey

oadiguzel@firat.edu.tr

Shape memory alloys take place in a class of functional materials by exhibiting a peculiar property called shape memory effect. This property is characterized by the recoverability of two certain shapes of material at different conditions. Shape memory effect is based on a solid state phase transition, martensitic transformation, which occurs with cooperative movements of atoms on cooling from high temperature parent phase region. Martensitic transformation occurs with lattice invariant shears which occur in {110}-type opposite directions on the {110}-type planes of austenite matrix. The basic processes are the twinning and detwinning in shape memory alloys. Thermal induced martensite occurs as twinned martensite, and the twinned structures turn into the detwinned structures by deforming the material in the martensitic condition. The deformed material recovers the original shape on heating over the austenite finish temperature, and cycles between the deformed and original shapes on cooling and heating, respectively, whereas the crystal structure cycles between the twinned and ordered parent phase structures. Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures at high temperature parent phase field, and these structures martensiticaly turn into the layered complex structures with lattice twinning on cooling. In the present contribution, x-ray diffraction, transmission electron microscope and differential scanning calorimeter (DSC) studies were carried out on two copper based ternary alloys. The x-ray diffractograms taken in a long time intervals from the aged specimens at room temperature reveal the structural changes in diffusive manner.

The hydrogen solubility in silicates at high pressure

Efimchenko V S[@], Galitskaya Y A, Fedotov V K, Meletov K P and Barkovskii N V

Institute of Solid State Physics of the Russian Academy of Sciences, Institutskaya Street 2, Chernogolovka, Moscow Region 142432, Russia

[@] efimchen@issp.ac.ru

The solubility of molecular hydrogen in silicate glasses containing magnesium (which is a parameter important for Geology and Earth Geophysics), and in crystalline forsterite at a hydrogen pressure of 5.5 GPa and temperature 250 °C was first studied by the method of thermobaric quenching. The highest molar ratio X = H_2/f.u. = 0.35 was obtained for the amorphous phase $Mg_{0.6}SiO_{2.6}$. The solubility of hydrogen in the amorphous forsterite Mg_2SiO_4 with the maximal Mg content was slightly lower and amounted to X = 0.23. The hydrogen solubility in the crystalline forsterite under the same conditions was lower by the order of magnitude and equal to X = 0.035.

A comparison of hydrogen solubilities in the forsterite glass and in the quartz glass at 5.5 GPa and 250 °C shows that magnesium halves the hydrogen content of the glass from X = 0.48 for SiO_2 down to X = 0.23 for Mg_2SiO_4. An investigation of the quenched samples by Raman spectroscopy shows that hydrogen in the amorphous $Mg_{0.6}SiO_{2.6}$ is dissolved in the form of H_2 molecules that manifests itself by a band of stretching H-H vibrations at a frequency of 4180 cm^{-1}. The band of stretching vibrations of H_2 molecules dissolved in the crystalline forsterite is shifted to 4155 cm^{-1}. In addition to this band, the Raman spectrum of the hydrogenated forsterite shows a peak at 915 cm^{-1}. The most likely origin of such a peak is vibrations of strong Mg-H bonds formed by a considerable fraction of the dissolved hydrogen. The hydrogen in the crystalline forsterite is therefore expected to exist both in the molecular and atomic forms.

The behavior of boron carbide under non-hydrostatic stress

Korotaev P Yu[@], Pokatashkin P A and Yanilkin A V

All-Russia Research Institute of Automatics named after Dukhov, Sushchevskaya 22, Moscow 127055, Russia

[@] korotaev@vniia.ru

In the question of boron carbide's application as structural material probably most important point is its behavior under stress. Partially, the series of phase transitions during shock-wave loading is still not well understood [1, 2]. We use quantum molecular dynamics simulations to reveal the stability of boron carbide structure under non-hydrostatic stress. The simulations show that under non-hydrostatic stress boron carbide exhibits two structural phase transitions, which activation depends upon direction of deformation and its value. The equation of state of quasi-hydrostatic loading was obtained [3]. Above critical value of deformation normal to three-atomic chain abrupt chain bending occurs, leading to change in stress components. When activated locally, this structural change can explain the series of phase transitions above 35 GPa during shock-wave loading. The second structural transition is the disordering of the structure, leading to relaxation of non-hydrostatic stress.

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Experimental investigation of thermophysical properties of carbides of refractory metals at high temperatures

Senchenko V N[1], Belikov R S[1,2,@], Popov V S[1,2] and Melnikov S A[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] roman.belikov@phystech.edu

Using the experimental setup for investigation of the thermophysical properties of refractory carbides under high pressure and temperature a few experiments with the different materials were carried out. Experiments with the eutectic composition of MoC–C have demonstrated that the installation allows obtaining data on the specific enthalpy, heat capacity, electrical resistivity and thermal expansion of various carbide-like systems. Our approach allows adjusting the heating rate in a wide range from 10^6 to 10^8 K/s at a high static pressure [1]. The high speed shadowgraphy allows measuring of the dependence of linear expansion of the material during its heating and melting. Dependences of the specific heat and enthalpy, electrical resistivity and specific expansion of the eutectic composition MoC–C obtained in the experiments are in a reasonable accordance with the available literature data for stoichiometric carbide Mo_2C. Dependence of the electrical resistance which is untypical for other carbides of refractory metals was experimentally confirmed [2], and the value of the heat of fusion of this material was for the first time obtained. Because of its absence the literature data for the eutectic composition in the entire temperature range and, for the stoichiometric composition, near the melting point are of great interest.

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High-speed multichannel pyrometer for high temperatures properties investigations

Senchenko V N[1], Belikov R S[1,2] and Popov V S[1,2,@]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] SlavaPopov1991@yandex.ru

An experimental setup allows one to investigate thermal properties of refractory conductive materials in the pre-melting region and in the liquid phase with high accuracy.
The experimental technique is based on rapid resistive self-heating of the specimen up to the melting temperature in a short period of time (25–600 μs) by passage of an electrical current pulse through it. Thus, by measuring the surface temperature of the specimen during the experiment, current and voltage between the potential probes in the middle part of it one can determine the temperature dependence of enthalpy and specific heat of material.
For the high-speed measurement of the specimen temperature a special four channel pyrometer was created. Temperature measurements are carried out in a narrow bandwidth of about 25 nm in the wavelength range 650–1050 nm. The narrow spectral bandwidth of a monochromatic provides a constancy of effective wavelength in a wide temperature range of 1300–7000 K. The pyrometer target is a circular area 0.3 mm in diameter. In order to provide a long-term stability of measurements the photodiodes are placed inside the box with a temperature keeping constant by means of a positive thermostat with an accuracy of 0.1 K. Pyrometer was calibrated in the temperature range 1773–3273 K using high temperature blackbody model. The relative error of the pyrometer calibration does not exceed 0.25%.

Temperature determination in an isothermal system of opaque bodies from a thermal radiation spectrum

Rusin S P

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

sprusin@yandex.ru

The thermodynamic (true) temperature determination from a thermal radiation spectrum in an isothermal system of n opaque heated bodies is considered. All the bodies have the same thermodynamic temperature and are in the diathermic environment. Since the opaque bodies, it is convenient to consider radiation heat transfer between the surfaces of these bodies. It is assumed that the emission and reflection surfaces depending on the direction. An analysis of the radiation heat transfer carried out via optical-geometric functions that characterize the transfer of radiation from one surface element to another directly and as the result of multiple reflections in the system. It is shown that for an isothermal system of emitting bodies this problem is identical to the definition of the true temperature of a free-radiating body [1]. In this case, it should be replaced the emissivity of the material freely-radiating object on the effective emissivity. The relationship is obtained for the isothermal system of opaque bodies, which relates a wavelength of maximum spectral radiation of the system, the effective spectral emissivity of the system and its thermodynamic temperature. In the particular case of a black or gray radiation, this relationship identically the Wien displacement law. The ability to determine the thermodynamic temperature of the system with the help of the resulting relationship is discussed.

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Investigations of thermal conductivity of metals in the field of centrifugal and vibration accelerations

Lepeshkin A R[@] and Vaganov P A

Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

[@] lepeshkin.ar@gmail.com

The investigations of the thermal conductivity of a metals in the field of action of the centrifugal and vibration accelerations is a new work which is important for aerospace engineering. The turbine blades operate at centrifugal accelerations of 4000–10000 g and vibration accelerations 100–1000 g and we can expect significant thermoconductivity change in these conditions. In the work the methods and devices for investigations of thermal conductivity of materials in the field of centrifugal radial and district and vibration accelerations have been developed. From the analysis of the results of experimental investigations it may be stated that the thermal conductivity of the heat-conductors increases significantly with an increase of a rotation frequency or amplitude of oscillations (with an increase of the electron drift velocity) compared to the steady state. The obtained results are of practical importance for the assessment of the thermal state of the rotating parts of aircraft engines and other energy turbomachines.

Thermodynamic properties of vanadium and cobalt argide ions, VAr^+ and $CoAr^+$

Maltsev M A[1,2,@], Kulikov A N[1] and Morozov I V[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] daerus21@yandex.ru

The compounds of 3d metals and the ions of argon Ar^+ (metal argides, MAr^+) play essential role in the mass spectrometry with argon plasma sources. At the same time their thermodynamical properties are still not sufficiently studied. Rough estimations of the internal partition functions of MAr^+ has been made in [1] which is needed to calculate the concentration ratio between metal and metal argide ions in the plasma.
We performed more accurate calculations of the internal partition functions for VAr^+ and $CoAr^+$, for which the experimental measurements of molecular constants are available. The partition functions and equilibrium constants were obtained for the temperatures up to 20 kK. The molecular constants were used to construct the potential curves for the ground and excited states of the molecules. The one-dimensional Schrodinger equation was solved using the Level code (version 8.2) [2] to find the vibration-rotational levels of the electronic states for the specified potential. Different potential models such as a simple Morse potential and the potential with the long range electrostatic attraction [3] were used for comparison.

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Equation of state of fluid monolayer absorbed on a stochastic surface

Khlyupin A N[1,2,@] **and Dinariev O Y**[2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
[2] Schlumberger Moscow Research Center, Pudovkina 13, Moscow 119285, Russia

[@] khlyupin@phystech.edu

We consider the lattice gas approach to statistical mechanics of fluid adsorbed on random surfaces with fluid–fluid and fluid–surface potentials. It was shown that effective Hamiltonian contains quenched random interactions and random site fields. Their statistical features combine the properties of random geometry and fluid–fluid pair interaction potential.
The first and the second terms in high-temperature expansion lead to Scheider–Pytte Random Field Ising Model (RFIM) [1] and Sherrington–Kirkpatrick (SK) Spin-Glass model [2] with infinite-ranged independently distributed random interactions, respectively. Equation of state and thermodynamic properties are evaluated using replica theory procedure in replica symmetric ansatz.
On the other hand we consider the Random Field model in random graph with finite connectivity instead of previous "infinite-ranged" approximations. This model has been investigated using finite connectivity technique introduced in [3,4]. The replica symmetry ansatz for the order function is expressed in terms of a two-dimensional effective-field distribution, which is determined numerically.

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Synthesis and thermal properties of pristine and hydrogenated carbon graphene-like materials

Tarala V A[1], Akhmatov Z A[2] and Khokonov A Kh[2,3,@]

[1] North-Caucasus Federal University, Pushkina 1, Stavropol 355009, Russia
[2] Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia
[3] Institute for Nuclear Research of the Russian Academy of Science, Prospekt 60-letiya Oktyabrya 7a, Moscow 117312, Russia

[@] ahmatov.z@bk.ru

Different kinds of graphene-like samples were manufactured by methane-hydrogen mixture deposition (CVD) on sapphire substrate. Various pure carbon nanostructures such as pristine graphene, graphyne, multilayer graphene and hydrogenated graphene e.g. graphane were obtained. Structures identification have been done by Raman spectrometry by comparison intensities of D, G, and 2D peaks lying at frequencies 1350, 1580, 2690 cm^{-1} correspondingly. Lattice dynamic namely phonon dispersion laws and density of state were studied in the frame of analytical models [1] and program for quantum-chemical simulation HyperChem. Electronic band structure and the influence of hydrogenation degree on the gap width between valence and conductivity zones for graphene-like 2D lattices were studied by means of LCAO MO method [2]. Possible superconductivity in multilayer graphane [3] and metal intercalated multilayer graphene are discussed [4, 5].

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About application of derivatives of fractional order to taking into account the principle of local disequilibrium

Magomedov R A[@], Meilanov R P, Akhmedov E N and Aliverdiev A A

Institute for Geothermal Research of the Daghestan Scientific Center of the Russian Academy of Sciences, Shamil 39a, Makhachkala, Daghestan 367030, Russia

[@] ramazan_magomedov@rambler.ru

Here we have presented the generalization of thermodynamics in formalism of fractional derivatives [1]. The Boltzmann–Gibbs thermodynamics results are obtained for particular case, when the rate of derivative of fractional order $\alpha = 1$. We have obtained the one-parametric "fractal" state equation with second virial coefficient. We have shown that transition from standard derivatives to derivatives of fractional order represents the technique of accounting of the local non-equilibrium concept, when the thermodynamic process is affected by fluctuations of the thermodynamic parameters [2]. As a particular application of the "fractal" state equation we have considered P, V, T—properties of neon Ne (as single-component compound), three-component refrigerant R409B (freon) and calculated compressibility factor, coefficients of van der Waals, entropy. Obtained results satisfactorily coincide with the experimental data of other authors. The opportunity of application of the "fractal" state equation for the extreme state research is discussed.
The work was partially supported by RFBR (16-08-00067a).

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Neuromorphic approach for information processing of image reconstraction

Manykin E A[1,2,@], Grichuk E S[1] and Kuzmina M G[3]

[1] National Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia
[2] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[3] Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, Miusskaya Square 4, Moscow 125047, Russia

[@] edmany@mail.ru

A neuromorphic adaptive method of information processing for problems of brightness image segmentation (reconstruction) has been developed. The method is based on controllable cluster synchronization in spatially two-dimensional oscillatory network model. The modification Ginzburg–Landau oscillator is chosen as single network oscillator. Oscillatory network performance imitates the known phenomenon of synchronization-based dynamical binding, that is presumably used by a number of the brain neural structures during their performance. The developed oscillatory-network approach demonstrates the following capabilities: high quality segmentation of real grey-level and color images; selective image segmentation (exclusion of unnecessary information); solution of a problem of visual scene segmentation—the problem of successive selection of all spatially separated image fragments of almost equal brightness. A model of a system of stochastic oscillators has been designed as well. The initial results on modeling of classical analogy of mixed quantum entangled state (that is usually considered as a resource of one-way quantum computations) have been obtained [1].

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Bifurcation of viscous fluid flow in a channel with sudden contraction and expansion

Kravchenko I V[1] **and Patlazhan S A**[2,@]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] Semenov Institute of Chemical Physics of the Russian Academy of Sciences, Kosygina 4, Moscow 119991, Russia

[@] sapat@yandex.ru

Viscous fluid flow in 2D channel with the sudden constriction and expansion was investigated by means of numerical modeling. The fluid motion was induced by pressure drop and simultaneous movement of pistons on each side of the narrow part of the channel. In both cases attention was focused on regularities of transition from axisymmetric flow pattern to the steady-state asymmetric flow in the expansion zone of the channel. This bifurcation was found to be caused due to the spontaneous symmetry breaking of dimension of the lateral vortices and takes place at Reynolds numbers above a certain critical value. The flow asymmetry appeared within a time lag after beginning of flow. The delay was shown to increase with approaching to the critical Reynolds number. Degree of flow asymmetry was described in terms of difference between dimensions of the lateral vortices relative to their values in a symmetrical flow mode. It was found that this characteristic is linearly dependent of Reynolds number. Comparative study of pressure and piston driven flows was carried out.

Hydrodynamics of power-law fluid in microchannel with superhydrophobic wall

Vagner S A[1,@] **and Patlazhan S A**[2]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] Semenov Institute of Chemical Physics of the Russian Academy of Sciences, Kosygina 4, Moscow 119991, Russia

[@] vagnerserge@gmail.com

Flow peculiarities of the Carreau–Yasuda power-law fluid past anisotropic superhydrophobic (SH) representing array of parallel microgrooves were studied by means of numerical simulation. The fluid is assumed does not penetrate into the groves of SH wall and results in the effective slip. The origin of the slippage length is discussed. We found that shearing of the non-Newtonian fluid results in formation of the low-viscous layer in the vicinity of SH wall which reduces significantly the hydrodynamic resistance of a microchannel. The effective slippage length of the Carreau–Yasuda fluid was shown to be significantly larger than that of Newtonian fluid. If the SH texture is oriented at some angle to the channel axis, the stream lines was found to deviate from the axis resulting in generation of the transversal secondary flow thus contributing to the helicoidal flow. The deviation angle of stream lines was found to decrease in the case of the power-law fluid as compared with the Newtonian one. The influence of SH texture and channel parameters to deviation angle and slippage length of the Carreau–Yasuda power-law fluid was investigated.

The viscosity and surface tension of nuclear matter and quark-gluon plasma

Khokonov A Kh[1,2]

[1] Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia
[2] Institute for Nuclear Research of the Russian Academy of Science, Prospekt 60-letiya Oktyabrya 7a, Moscow 117312, Russia

azkh@mail.ru

In present the interest to nuclear matter hydrodynamics increases [1]. Liquid drop model (LDM) successfully being used for semi-empirical formulation of surface and Coulomb terms in Bethe-Weizsacker mass formula. LDM is foundation for 5D harmonic oscillator collective nuclear model [2], which allows to interpret vibration excitations of near-spherical nuclei. In the frame of nuclear liquid drop model an analytical solution for the frequency of capillary oscillations is obtained with taking into account the damping due to viscosity and surrounding medium polarizability. The model has been applied for estimation of even-even spherical nuclei surface tension and viscosity. It has been shown [3, 4] that energy shift of capillary oscillations of even-even spherical nuclei due to viscous dissipation gives viscosities in the interval 4.2—7.6 MeV fm^{-2} c^{-1} for nuclei from Pd—106 to Hg—198. For non zero temperatures the ratio of shear viscosity η to entropy density s is estimated and compared with the limit $\eta/s > 1/4\pi$ motivated by AdS/CFT for quark-gluon plasma [5].

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Molecular-dynamics modeling of phase transformation in copper under shock conditions

Bolesta A V[1,2,@] **and Fomin V M**[1,2]

[1] Institute of Theoretical and Applied Mechanics of the Siberian Branch of the Russian Academy of Sciences, Institutskaya 4/1, Novosibirsk 630090, Russia
[2] Novosibirsk State University, Pirogova Street 2, Novosibirsk 630090, Russia

[@] bolesta@itam.nsc.ru

At extreme pressures and temperatures common materials form new dense phases with compacted atomic arrangements. By classical molecular-dynamics simulation, we observe that fcc copper undergo phase transformation to bcc structure. The transition occurs under shock wave loading at the pressures above 100 respectively, and corresponding temperatures above 2000 K. We calculate phase diagram, show that at these pressures and low temperature fcc phase of copper is still stable and discuss the thermodynamic reason for phase transformation at high temperature shock wave regime.

Numerical simulation of the high-speed impact of two metal plates

Fortova S V[@], Shepelev V V, Pronina A P and Utkin P S

Institute for Computer-Aided Design of the Russian Academy of Sciences, Vtoraya Brestskaya 19/18, Moscow 123056, Russia

[@] sfortova@mail.ru

On the basis of the numerical simulation dynamic processes occurring in the high-speed impact of the two metal plates are investigated. The calculations showed the presence of the Rayleigh–Taylor instability, growing at the impact boundary metals. The comparative characteristic of the metal deformation processes in the spatial case with different equations of state is given.

Equation of state of aluminum consistent with molecular dynamic potential

Krasnova P A[@], Levashov P R and Povarnitsyn M E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] pakrasnova@gmail.com

Modern supercomputers allow one to perform atomistic simulations with more than 10^9 particles. This opens the possibility to study different macroscopic properties and processes on the atomic level. In particular, hydrodynamic instabilities, shock and detonation waves, heat conductivity and diffusion may be studied by molecular dynamics in a region with a characteristic size of several microns. On the other hand, continuum mechanics simulations with an equation of state (EOS) are required in the case of a bigger computational domain. Obviously, thermodynamic properties given by the EOS and a molecular dynamic potential should be consistent with each other. This is especially important for hybrid approaches in which both microscopic and macroscopic simulation is applied. In this work we present the EOS of Al consistent with the embedded atom potential [1]. This potential is in agreement with available experimental data and first-principle calculations and can be used at high pressures and moderate temperatures. The phase boundaries of solid–liquid and liquid–gas transitions were calculated earlier by the two-phase method [2]. We perform MD computations of different thermodynamic properties in the isothermal and isobaric ensembles on a triangular grid of points in each phase state and then interpolate the results. The EOS is available in a tabular form.

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Nucleation and spall strength of liquid metals

Lopanitsyna N Yu[1,2,@] **and Kuksin A Yu**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] lopanitsyna@phystech.edu

Under the action of high energy density fluxes the melting of metal is probable and fracture starts in a liquid phase. However, the models for description of fracture kinetics in such a conditions, reached just for a short time, are hard to verify experimentally.
This work is aimed to study of metastable liquid metals under tension by means of atomistic simulations and to develop a model describing a tensile fracture of melts. Systems with various surface tension are analysed: liquid Al, Fe, Mo. Nucleation rates are calculated from molecular dynamics simulations [1] basing on the average lifetime of the metastable state until formation and growth of cavity. The data on nucleation rate are approximated in the form of nucleation theory [2]. It is shown that correct description is achieved if curvature dependence of surface tension (the Tolman's correction) is taken into account. Tolman's length has a different value for different model systems. A correlation between the Tolman's length and the surface tension (on a plane boundary) is detected.
The overall model of fracture is based on nucleation and growth approach. The spall strength could be calculated from these considerations using surface tension, viscosity and data on the equation of state of melt. The obtained results for Mo and Al are consistent with experimental data [3] and direct MD calculations at strain rates $\approx 10^{10}$–10^{11} s^{-1}. Comparison with the estimates of spall strength of Sn at low strain rates from [4] is discussed.

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Diffusion of vacancies in bcc metals and its dependence on temperature

Fidanyan K S[1,2,@] **and Stegailov V V**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] fidanyan@phystech.edu

The motion of defects in the uranium lattice is important for the study of radiation damage, because the mechanical and conductive properties of the material change with the accumulation of such defects.

The generally accepted model for temperature dependence of diffusion of defects is the Arrhenius equation $D = D_0 \exp[-E_a/k_B T]$, where E_a is a potential energy barrier and D_0 is a frequency factor, determining an effective frequency of jump attempts [1]. However, there is some evidence that the Arrhenius law is not accurate at high temperatures, when anharmonicity of atomic interactions can not be neglected and makes a significant contribution to the formation and migration energy of defects [2]. Researchers also discuss temperature effects on the vacancy formation volume and consecutive effects on the mobility of vacancies [3].

This work shows that the molecular dynamics simulation of the motion of defects in bcc metals reveals the deviation from the Arrhenius law. Temperature dependence of the migration energy is discussed, and the new techniques for evaluation of the pre-exponential factor are considered.

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Molecular dynamics study of viscosity during glass transition of aluminum melt

Kirova E M[1,2,@] and Pisarev V V[2,1]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] kirova@phystech.edu

The liquid-glass transition is one of the most interesting question of the physics of amorphous state. Molecular dynamics study of shear viscosity behavior of liquid aluminum is carried out. The embedded atom method potential is used at the simulation of isobaric cooling [1]. The viscosity is calculated using the Green–Kubo formula. In the initial configuration atoms take a half the volume of simulation box as a film, parallel to the XY plane.
The dependence of the shear viscosity coefficient on temperature is obtained in the range 300–1200 K. In this paper, two different transition temperatures are detected. The first one corresponds to the change of stress autocorrelation function (SACF) with components along the Z direction. The function shows oscillating behavior. The second one is characterized by "freezing" of SACF, ie, preservation of shear stress in the XY plane. A comparison of the results with the other numerical experiments is obtained [2]. Also, the kinematic viscosity is compared with the experimental data [3] for the temperatures above the melting temperature. Simulations are performed using the LAMMPS MD software [4].

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Nucleation of carbon nanostructures: Molecular dynamics with reactive potentials

Galiullina G M[1,2,@], Orekhov N D[1,2] and Stegailov V V[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] gulnaz_g@inbox.ru

Carbon compounds are very important part of everyday life. Therefore, the study of carbon structures is an interesting challenge for researchers during many years. In this paper we make an attempt to explore the details of carbon nucleation using computer simulation with molecular dynamics methods. That could predict thermodynamical conditions (pressure, temperature, density, etc) which would be the most appropriate to obtain ordered carbon compounds in an industrial scale.

Simulations were conducted with reactive potentials ReaxFF (Reactive Force Field) [1] and AIREBO [2]. Reactive nature of potentials takes into account the breaking and the formation of bonds due to the inclusion in the model short-range and long-range forces. Thus, calculations have quantum mechanical precision without requiring such computational resources as ab initio ones.

The influence of the interatomic potential on the nucleation of ordered structures in the gas phase was analyzed on the base of different seeds. Simulations are performed with program package LAMMPS [3].

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Tensile strength of Al matrix with nanoscale Cu, Ti and Mg inclusions

Pogorelko V V[@] and Mayer A E

Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia

[@] vik_ko83@mail.ru

With the use of the molecular dynamics simulations we consider three different mechanisms of reduction of the tensile strength of a material with inclusions in comparison with a pure material of matrix. The first mechanism is connected with a stress concentration in matrix near a stiff and strong inclusion (Ti, Cu); in this case, the fracture occurs inside the matrix and does not touch the inclusion. The second mechanism acts in the case of a soft and weak inclusion (Mg); the fracture begins inside the inclusion and thereafter propagates into the matrix.

The tensile strength of Al+Cu, Al+Ti and Al+Mg systems is determined at varied strain rates (in the range from 0.1/ns to 30/ns at the temperature 300 K) and varied temperatures (in the range from 300 K to 900 K at the strain rate 1/ns). The rate sensitivity of strength of a material with inclusions is higher than that for a material without inclusions. Temperature dependences of tensile strength are qualitatively different for the systems Al+Ti and Al+Mg.

We propose a continuum model of the nanocomposite fracture that is based on the equations of nucleation and growth of voids; the model takes into account the stress concentration around inclusions. A comparison with the MD results shows that the continuum model allows us to describe the rate and temperature dependences of the nanocomposite strength at least for strain rates ≥ 0.1/ns. At moderate strain rates, the strength values that are calculated with the continuum model correspond to the experimental data for the aluminum alloy 2024 with the second phase precipitates.

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Effect of sharp maximum in ion diffusivity for liquid xenon

Lankin A V[1] **and Orekhov M A**[2,1,@]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] mo2411@mail.ru

Ion diffusion in a liquid usually could be treated as a movement of an ion cluster in a viscous media [1–4]. For small ions this leads to a special feature: diffusion coefficient is either independent of the ion size [4] or increases with it [2]. We found a different behavior for small ions in liquid xenon.

Calculation of the dependence of an ion diffusion coefficient in a liquid xenon on the ion size is carried out. Classical molecular dynamics method is applied. Calculated dependence of the ion diffusion coefficient on its radius has sharp maximum at the ion radius 2 Å. It is placed between two stable ion cluster configurations. This leads to the instability of both of them in a small region between them. Consequently ion with radius near 2 Å could jump from one configuration to another. This increases the diffusivity of the ion.

Diffusion coefficient in the area of stable ion clusters is in agreement with the model [1]. According to this model there are no dependence of diffusion coefficient on the ion radius.

The sharp maximum is in a good agreement with experimental value [1] of O_2^- diffusion coefficient in liquid xenon.

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Development of new atomistic model of Zr and Zr-Nb alloys for study of structure, phase transitions and diffusion properties

Starikov S V[1,2,@], Smirnova D E[1] and Gordeev I S[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] starikov@ihed.ras.ru

A new attempt to study properties of Zr-Nb structural alloys is reported. For this purpose a new angular-dependent many-body interatomic potential is constructed. The potential functions have been fitted towards the *ab initio* data computed for a large set of reference structures. Description of the fitting procedure is given and its accuracy is discussed. It is shown that the structure and properties of all Nb and Zr phases existing at the Zr-Nb phase diagram are reproduced with a good accuracy. Especially it is worth noting that the potential presented is appropriate for study of high-pressure hexagonal ω-phase of Zr. In addition, created potential allows to study Zr melting line that is important due to the lack of the corresponding experimental data. Characteristics of the point defects in α-Zr, β-Zr and Nb are also estimated and are proven to correlate with the existing experimental and theoretical data. In case of hcp structure the model reveal anisotropy of defects diffusion, in agreement with previous calculations. The potential provides an opportunity for simulation of Zr-Nb alloys based on α-Zr and β-Zr.

Features of structure and phase transitions in pure uranium and U-Mo alloys: Atomistic simulation

Kolotova L N[1,2,@], Kuksin A Yu[1,2], Smirnova D E[1], Starikov S V[1,2] and Tseplyaev V I[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] lada.kolotova@gmail.com

Uranium has received a lot of attention due to its unique nuclear properties and its various applications in nuclear industry. In order to improve mechanical properties and corrosion resistance of uranium at room temperature while maintaining the high density, uranium is frequently alloyed with the other metals. Compared with the other high density uranium alloys and compounds, the low-enriched uranium alloys with 6–12wt.% of Mo have attracted a great deal of attention and are recognized as the most prominent candidates for advanced research and test reactors.
One should note that pure uranium has three different phases depending on temperature and pressure. Therefore, structure of uranium-based alloys (namely, U-Mo) can reflect features of different uranium phases, depending on conditions. The structural properties of body-centered cubic (BCC) and body-centered tetragonal (BCT) phases of pure uranium and U-Mo alloys are studied using atomistic simulations. The BCC lattice exhibits cubic symmetry only on the scale of several interatomic spacings, and it is therefore more correct to denote the high-temperature state of pure uranium and U-Mo alloys as quasi-BCC. The local positions of uranium atoms in the quasi-BCC phase correspond to the BCT structure. This fact is the possible origin of the difficulties encountered in the description of the BCC phase of pure uranium by *ab initio* methods that has been a challenge for researchers for decades.

Atomistic simulation of a superionic transition in fluorite type structures UO_2, UN_2, TiH_2

Korneva M A[@] and Starikov S V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] marijakorneva@yandex.ru

It is known that fluorite type structures can show superionic transition at high temperatures. Since 1990 there were series of experiments and calculations that proved the existence of such transition in some of these structures. One of characteristics of this process is high growth of conductivity (both electric and heat).
There are certain difficulties in constructing the theory of superionic transitions. There still remain a number of fundamental questions: whether the superionic transition actually can be considered as a phase transition, to which type this phase transition belongs, what is the mechanism of this transformation, and what are the necessary conditions for the observation of this transition (so far, there is no evidence to suggest that the superionic transition can be observed in all structures of the fluorite type).
In this work the results of the atomistic simulation of a superionic transition and melting of stoichiometric UN_2, UO_2 and TiH_2 have been presented. The first structure didn't show superionic transition, while others did. The temperature dependences of defects concentration in the anion sublattice and leaps of the heat capacity and isothermal compressibility have been calculated in UO_2 and TiH_2. To obtain phase diagrams all three systems were studied in a wide range of temperatures and pressures. It has been shown that the curve of the superionic transition in the P–T-diagram can be described by the Ehrenfest equation. The possibility of describing the superionic transition within the framework of the theory of second-order phase transitions has been discussed. The conditions of the existence of superionic transition have been discussed.

The effect of strain on hydrogen diffusion barriers in bcc iron: Molecular dynamics study

Emelin D A[1,2,@] **and Mirzoev A A**[1]

[1] South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia
[2] Federal State Unitary Enterprise "Russian Federal Nuclear Center—Academician Zababakhin All-Russian Research Institute of Technical Physics", Vasilieva 13, Snezhinsk, Chelyabinsk Region 456770, Russia

[@] emelin_d_a@mail.ru

The negative effects of hydrogen on metals are strongly dependent on the specific features of hydrogen diffusion in specific materials. The dependence on hydrogen diffusion coefficient on material temperature and applied stress is of special value for the prediction of degradation in industrial products with substantial residual stresses (welded pipes, welds, bearing beams etc). In defectless bcc iron, hydrogen is known to reside at tetrahedral (T) sites. But under some temperatures and strains the equilibrium position od hydrogen can change from a tetrahedral to octahedral (O) site. This transition depends on the diffusion barriers which control hydrogen transition from a T-site either to the nearest neighbor T-site (T-S-T path), or to a T-site by crossing an O-site (T-O-T path). The dependence of the diffusion barriers on biaxial strains is of special interest in this context. The paper presents molecular dynamics calculations with EAM potential by Carter [1] for the dependence of the hydrogen diffusion barriers on hydrogen biaxial strains in defectless bcc iron. It has been shown that in a sample with dissolved hydrogen compressed above 7% and tensile 8% the diffusion barrier of the T-O-T transition is lower than that of the T-S-T transition. This outcome is indirectly confirmed by experiment [2] and was for the first time observed in DFT calculations [1, 3]. It is a basis for further studies into the diffusion hydrogen dissolved in deformed bcc iron.

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Influence of three body potentials on equations of state in the frame molecular dynamics

Akhmatov Z A, Khokonov A Kh and Khokonov M Kh[@]

Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia

[@] khokon6@mail.ru

Equations of state of inert gases and their mixtures in 3D volume as well as on 2D surface of (0001) graphite have been obtained in the frame of molecular dynamics method developed with account of three-body interactions. The energy of three body interaction $\Phi^{(3)}_{\rm ijk}$ is expressed through six algebraically independent polynomials of the transformation group $O(3) \times S_3$. Polynomials are comprised by radius-vectors joining the particles $r_{\rm ij} = |\mathbf{r_i} - \mathbf{r_j}|$ [1]. In this work, we used the LAMMPS program for multiprocessor MD computations along with the original program of MD modeling [2].
We utilize the following approximation of three body potential

$$\Phi^{(3)}_{\rm ijk} = \sum_{\{ijk\}} \left(\frac{Q_2}{I_1^6} - \frac{Q_1}{I_1^3} \right) + \frac{C}{I_3^{3/2}} \left(1 + \frac{3(\mathbf{r}_{\rm ij}\mathbf{r}_{\rm kj})(\mathbf{r}_{\rm ik}\mathbf{r}_{\rm jk})(\mathbf{r}_{\rm ij}\mathbf{r}_{\rm ik})}{I_3} \right)$$

where $I_1 = r^2_{\rm ij} + r^2_{\rm jk} + r^2_{\rm ki}$, $I_3 = r^2_{\rm ij} r^2_{\rm jk} r^2_{\rm ki}$ are invariants of use. The second term corresponds to Axilrod–Teller polarization potential [3]. Simulation carried out with Kob–Andersen binary mixture of krypton and xenon has shown the effect of component-wise exfoliation for evolution times exceeding significantly the times between individual interactions. It has been shown, that noticeable effect of three body interaction on values of critical pressures and temperatures takes place for heavy inertial gases characterized by higher polarizability.

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Rheology of liquid n-alkanes: Molecular dynamics calculation

Kondratyuk N D[1,2,@], Norman G E[1] and Stegailov V V[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] kondratyuk@phystech.edu

Modern industry is strongly interested in rheological properties of hydrocarbon liquids as main constituents of oils and fuels. The calculation of the transport coefficients for monoatomic systems has become a routine process [1], but in the case of complex liquids the application of classical methods faces difficulties [2, 3].
The diffusion coefficient of n-triacontane ($C_{30}H_{62}$) is calculated using Einstein–Smolukhovsky and Green–Kubo relations. We use three different force fields: TraPPE-UA (united-atom) [4], DREIDING (all-atom) [1] and OPLS (all-atom, includes the Coulomb interaction) [3], for making sure that obtained results are not artefacts of a particular model. The $\langle \Delta r^2 \rangle(t)$ has a subdiffusive part ($\langle \Delta r^2 \rangle \sim t^{\alpha}$), caused by molecular crowding at low temperatures. Long-time asymptotes of $\langle v(0)v(t) \rangle$ are collated with the hydrodynamic tail $t^{-3/2}$ demonstrated for atomic liquids [7]. The importance of these asymptotes are discussed. Parameters that provide the compliance of Einstein–Smolukhovsky and Green–Kubo methods are analysed. Temperature effects on the diffusion process are also treated. We compare results obtained using both equations with experimental data. The application of modified Stokes–Einstein equation for shear viscosity of polymers is presented.
The work is supported by the RSF grant 14-19-01295.

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Phase diagram of a binary hydrocarbon mixture

Pisarev V V[@], Norman G E and Stegailov V V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] pisarevvv@gmail.com

Molecular dynamics simulations are used to calculate the phase diagram of methane+n-butane mixture. The TraPPE-UA [1], TraPPE-EH [2] and OPLS-AA [3, 4] forcefield models are compared.
All forcefield models reproduce the existence of retrograde condensation at 330 K. The TraPPE family forcefields are better in terms of reproducing the P-T-X-Y phase diagram of the binary mixture while the OPLS-AA forcefield gives densities closer to the experimental values.
The shift of the phase diagram in porous space is estimated. The example of slit pores with Mie potential is considered. 4 nm and 10 nm wide pores with two different sets of wall-molecule interaction parameters are studied. It is shown that the solubility of methane in butane does not change significantly in the pores, while the shift of vapor composition is observed. The shifts are stronger in the 4 nm pores than in the 10 nm pores. Such shifts in vapor composition lead to the increase or decrease of the critical point of mixture, depending on the wall-molecule interaction strength.
The work is supported by the Russian Science Foundation grant No. 14-50-00124

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Features of non-congruent phase transition in modified Coulomb model of the binary ionic mixture

Stroev N E[1,2,@] **and Iosilevskiy I L**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] nikita.stroev@phystech.edu

Non-congruent gas-liquid phase transition (NCPT) have been studied [1] in modified Coulomb model of a binary ionic mixture C(+6) + O(+8) on a *uniformly compressible* ideal electronic background /BIM(∼)/. The features of NCPT in improved version of the BIM(∼) model for mixture H(+1) + He(+2) on background of *non-ideal* electronic fermi-gas are the subject of present study. Analytical fits [2] for Coulomb corrections to EoS of electronic and ionic subsystems were used in present calculations within the Gibbs–Guggenheim conditions of non-congruent phase equilibrium [3]. Parameters of critical point-line and pressure and temperature end-point-lines were calculated on the entire range of proportions of mixed ions $0 < X < 1$. Strong "distillation" effect was found for NCPT in present BIM(∼) model. Just similar distillation was obtained in variant of NCPT in dense nuslear matter [4]. Absence of azeotropic compositions was revealed in studied variants of BIM(∼) in contrast to explicit existence of azeotropic compositions for the NCPT in chemically reacting plasmas and in astrophysical applications [4, 5].

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Theoretical model of the equation of state for calculation of ternary mixtures

Bogdanova Yu A[@], Gubin S A and Anikeev A A

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

[@] bogdanova.youlia@bk.ru

Obtaining the equation of a state (EOS) a multicomponent fluid plays an important role in creation of theoretical model of calculation of thermodynamic parameters of multicomponent systems. In this work the new effective two-fluid model based on the developed EOS of two-component fluid [1] is presented. In this model division of all components of mixture into two groups with close well-depth parameters is supposed. Thus, multicomponent mixture is presented in the form of an effective two-component fluid. This technique allows to avoid the mistake brought in calculation of thermodynamic parameters of multicomponent mixture with different well-depth of components of an effective one-fluid model [2]. The offered technique was applied to calculations of parameters of a condition of ternary mixture with various compositions of components in the range of moderate pressure and temperatures. Also the corresponding calculations with use of an effective one-fluid model [3] were carried out. Comparison of results of calculations with experimental data shows higher precision offered in this work an effective two-fluid model, than the vdW1f model. Research is executed at the expense of a grant of the Russian Science Foundation (project No. 16-19-00188).

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Experimental study of methane–n-pentane mixture filtration regimes

Zaichenko V M, Kachalov V V, Molchanov D A and Torchinskiy V M[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] torchvm@yandex.ru

The study results of filtration process of hydrocarbon mixtures of methane series in porous medium are presented in this paper. Interest in the filtration problem of such mixtures is aroused by the need to intensify production of heavy fractions of gas-condensate—valuable hydrocarbons, consisting of methane and its higher homologues. Different flow regimes including oscillatory one are observed during gas-condensate extraction under natural conditions [1]. The reason for these oscillations have remained unclear. Our studies have shown that there are multiple flow regimes under isothermal conditions for this type of mixtures depending on the initial pressure, the kind of the mixture's phase diagram and the permeability coefficients of the liquid and gas phases in the porous medium. Use was made of binary mixture methane–n-pentane as a model one. The critical pressure of the mixture is 18.5 MPa on the isotherm $T = 300$ K, and its phase diagram has a broader retrograde area compared with earlier investigated mixtures of methane–n-butane and methane–propane–n-butan [2]. The results of experimental studies of methane–n-pentane mixture filtration in porous medium under isothermal conditions in pressure range typical for gas-condensate reservoirs are presented.

This study has done within the program IV.4.14 of fundamental research of DPEMEMCP RAS.

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Mathematical modeling of gas-condensate mixture filtration in porous media, taking into account nonequilibrium phase transitions

Kachalov V V, Molchanov D A[@], Sokotushchenko V N and Zaichenko V M

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] dmitriy.molchanov13@gmail.com

Currently, a considerable part of the largest dry gas reservoirs in Russia are found in stage of declining production, therefore active exploitation of gas-condensate fields will begin in the coming decades. There is a significant discrepancy between the project and the actual value of condensate recovery factor while producing reservoir of this type, which is caused by insufficient knowledge of nonequilibrium filtration mechanisms of gas-condensate mixtures in reservoir conditions [1].

A system of differential equations to describe filtration process of two-phase multicomponent mixture for one-, two- and three-dimensional cases is presented in this work. The solution of the described system was made by finite-element method in the software package "FlexPDE". Comparative distributions of velocities, pressures, saturations and phase compositions of three-component mixture along the reservoir model and in time in both cases of equilibrium and non-equilibrium filtration processes were obtained. Calculation results have shown that system deviation from thermodynamic equilibrium increases gas phase flow rate and reduces liquid phase flow rate in filtration process of gas-condensate mixture.

This work was supported by the Russian Science Foundation (project No. 14-50-00124).

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Energy-technological complex with reactor for torrefaction

Kuzmina J S[@], Director L B and Zaichenko V M

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] juli_kuzmina@mail.ru

To eliminate shortcomings of raw plant materials pelletizing process with thermal treatment (low-temperature pyrolysis or torrefaction) can be applied [1]. The paper presents a mathematical model of energy-technological complex (ETC) for combined production of heat, electricity and solid biofuels torrefied pellets [2]. According to the structure the mathematical model consists of mathematical models of main units of ETC and the relationships between them and equations of energy and material balances. The equations describe exhaust gass straining action through a porous medium formed by pellets. Decomposition rate of biomass was calculated by using of grossreaction diagram, which is responsible for the disintegration of raw material [3]. A mathematical model has been tested according to bench experiments on one reactor module. From nomographs, designed for a particular configuration of ETC it is possible to determine the basic characteristics of torrefied pellets (rate of weight loss, calorific value and heat contents) specifying only two parameters (temperature and torrefaction time). It is shown that the addition of reactor for torrefaction to gas RIC engine can improve the energy efficiency of power plant. This work was supported by the Ministry of the Russian Federation for Education and Science (project No. 14.607.21.0032, unique identifier RFMEFI60714X0032).

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Experimental stand for investigation of two-phase filtration of multicomponent hydrocarbon mixtures

Molchanov D A, Pazyuk Yu V[@] and Torchinskiy V M

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] tightcookie@mail.ru

Experimental stand "Plast" is designed to investigate the case of one-dimensional filtration process of hydrocarbon fluids at temperature and pressure conditions of actual reservoirs. The configuration of the stand allows you to vary the pressure of the model mixture in the range of 1.280 bar, temperature—in the range of 285–400 K, to monitor the pressure distribution along the experimental section (ES), to control the pressure drop at ES and the flow rate of model mixture. Changing of described parameters makes it possible to obtain different filtration regimes of multicomponent hydrocarbon mixtures. The bypass line allows you to simulate a variety of physical impacts on the bottom-hole area, which alters the flow pattern significantly.

An account of the gas-condensate mixture filtration features is given. The techniques of two-phase filtration process simulation of multicomponent hydrocarbon mixtures in porous medium are presented.

Generalization of the dual porosity for modeling of oil shale production

Izvekov O Y

Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

izvekov_o@inbox.ru

Unconventional resources of hydrocarbons attract attention of scientists from around the world. Oil shale formations are characterized by significant organic content but ultra low permeability. The common way for modeling of oil production from the oil shale is the model of dual porosity. In this work a new continual model wich generalize the model of dual porosity, plasticity theory and damage mechanics is proposed. The model takes into account such as the well-known phenomenon as slip along natural fractures, change in permeability of system of natural fractures due to dilatancy, development of secondary fractures in low permeability matrix due to overpressure. For the study of common phenomenon in the oil shale formation after drilling the problem of circular well in flat reservoir was solved.

Limited evaporation technique for pore structure investigation of different materials

Vervikishko D E[@] and Shkolnikov E I

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vitkina-darya@yandex.ru

Development of pore structure research methods is actual objective in both fundamental and applied studies. For meso- and microporous bodies adsorption-structural methods are mainly used. They are based on measuring and analysis of adsorption isotherms. Static measurement methods of pure gases and vapors adsorption isotherms are considered "classic". However, complicity of interpretation in a number of low temperature adsorption cases as well as durability of measurement at facilities with micro weigh-scale cause attempts to develop new approaches and research methods.

The purpose of this paper is to describe the operational principle and some results received with the help of laboratory facilities created by the authors for research of nanoporous materials, based on the original adsorption dynamic method, called limited evaporation technique (LET). Its distinguishing feature is that measurements are carried out in dynamic regime, without defining or presetting adsorbent vapors pressure.

Modernization of the method allowed increasing its sensitivity in a zone of micropores with radius less than 1 nm. Detailed analysis in this zone is very important for many applications. Testing of a new design and opportunities of our device was held on activated carbon produced from wood waste. The main pore size is concentrated in the radius range 0.8–2 nm. These carbons are used in supercapacitors. Application of the LET allowed choosing optimum mode of activation and creating carbons that possess very high specific electric capacity. This is one example of using LET while creating or testing functional materials. LET allows making detailed analysis of pore structure of different materials.

The gravitationally neutral matter/antimatter universe-crystal with decelerative and accelerative expansion epochs

Gribov I A[1] **and Trigger S A**[2,@]

[1] Institute for Time Nature Exploration of the Moscow State University, Faculty of Biology, Division of General Ecology, Leninskiye Gory 1-12, Moscow 119991, Russia

[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] satron@mail.ru

A large-scale self-similar crystallized phase of the finite, gravitationally neutral universe (GNU)—a huge GNU-Ball—with spherical 2D-boundary, immersed into an endless empty 3D-space is considered. The main principal assumptions of this universe model are: (1) existence of stable elementary particles/antiparticles with the opposite gravitational charges ($M_{+\mathrm{gr}}$ and $M_{-\mathrm{gr}}$), which have the same postive inertial mass $M_{\mathrm{in}} = |M_{+\mathrm{gr}}| = |M_{-\mathrm{gr}}| > 0$ and equally presented in the universe during all universe evolution epochs; (2) the gravitational interaction between the masses of the opposite gravitational charges is repulsive; (3) the unbroken baryon-antibaryon symmetry; (4) M_+ and M_- charges symmetry, valid for two equally presented matter/antimatter GNU-components: (a) ordinary matter (OM)/ordinary antimatter (OAM), (b) dark matter (DM)/dark antimatter (DAM). The GNU-Ball is weightless crystallized "dust" of equally presented, mutually repulsive (OM+DM) clusters and (OAM+DAM) "anticlusters" [1,2]. Newtonian GNU-hydrodynamic gives the observable spatial flatness and ideal Hubble flow. The GNU in the obtained large-scale self-similar crystallized phase preserves its observable flatness, excludes the cluster/anticluster annihilation and explains the observable large-scale GNU phenomena.

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Calculation of the amplitude of acoustic oscillations arising from condensation of steam on liquid droplets

Pesochin V R

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

syrovatkara@gmail.com

Theoretical study of the excitation conditions of acoustic oscillations arising from condensation of steam on liquid droplets has been performed. We considered that the droplets are monodiperse and have a spherical shape. The Lewis number was assumed to be equal to unity. It was considered that specific heat capacity and thermal conductivity coefficient of molecular vapor mixture do not depend on temperature and concentration of the mixture components. The flow was assumed one-dimensional. The formulas for frequencies and the increment of the excitation of acoustic oscillations as well as their amplitude have been obtained.

The solution of the optimization problem of small energy complexes using simplex method

Ivanin O A[@] and Director L B

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] oleggin2006@yandex.ru

Schemes of small energy systems become more complicated: cogeneration and trigeneration schemes, schemes with heat and electric accumulators, hybrid circuits, including installations of renewable energy. These complexes usually provide energy for residential and social sector consumers, characterized by significant fluctuations of daily and seasonal loads. All this creates considerable difficulties in selecting the composition and characteristics of the equipment for energy complexes, its operation mode and control algorithms.
Solving this problem needs development of general-purpose mathematical models of energy complexes and up-to-date calculation programs. The necessity of long rated period (1 year) usage with small (1 hour) time step leads to great dimension of task and nonlinearity of characteristics makes its solution even more complicated. When using nonlinear optimization methods, the calculation time can be decades of hours.
For solving the optimization problem of small power energy complexes was adapted a method of linear optimization—the simplex method. The problem, formalized by system of balance equations for energy flows and corresponding linearized models of energy facilities, is reduced to a linear programming problem. The objective function being minimized is a linear functional, built on the criterion of energy supply cost. The constructed system of constraints reflects the physical essence of the problem. To reduce the dimension of the problem we consider the conditions of decomposition methods applicability. The results of comparative calculations for energy complexes of various configurations are presented.

Internet calculations of thermodynamic properties of substances: Results and problems

Ochkov V F[@], Ustyuzhanin E E and Shishakov V V

National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

[@] ochkov@twt.mpei.ac.ru

Internet resources with an information about thermodynamic properties, $R = (p, T, s \ldots)$, of technologically important substances are analyzed. Some functions and cloud templates for an Internet calculation of R properties of substances as well as the solutions of some applied thermophysical problems are considered. The experience of the authors [1] shows that the task is relevant to search for a software (SW) that makes it possible to adapt tabulated values of $R = (p, T, s \ldots)$ for a power plant (PP) design. The authors developed a specific technology and used a number of tools for the creation of SW that had a form of open interactive Internet (OI) resources ("IT functions", "cloud templates"). For example, OI resources were created and connected with such substances as H_2O, air, CH_4, Pb, Bi, Na, K, U, C, Cr and D_2O. A website NRU MPEI and a remote server were used. An important problem is the development and installation of SW in the form of OI resources those let to a designer to calculate the values of energy criteria, $Z = (Z_1$—a thermal efficiency, Z_2—a turbine power, Z_3—a heat input and other parameters of the cycle), with a respect to PP. For example, we have elaborated OI resource which is referred to as Code-1(Z, R, Y), where 1—a number of the code, $Y = (y_i)$—a set of border values including $Y = (p_1, T_1)$ those are the pressure and the temperature at the inlet of the first turbine, $R = (p, T \ldots)$—properties of the working body at predetermined points of the cycle. "IT functions" are involved in Code-1(Z, R, Y) and connected with R properties. A description of such OI resources is given in [1, 2].

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2. Shock Waves, Detonation and Combustion

Dynamics of shock and shockless compression waves in solids

Kanel G I

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

kanel@ficp.ac.ru

Brief overview will be presented of recent measurements of evolution of elastic-plastic compression waves in metals, glasses and ceramics under conditions of shock and gradient (shockless) loading. The shape, parameters and decay of elastic precursor waves in metals are controlled by the density of existing dislocations and by kinetics of their multiplication. In particular, non-monotonic decay of the elastic precursor wave in annealed vanadium, a change of kinetics of high-rate plastic deformation and corresponding shape of elastic precursor wave in copper with approaching the melting temperature, a deflection of evolution of elastic-plastic wave from self-similarity, unexpectedly large amplitudes of re-reflected wave at reverberation of an elastic wave between the free surface and the plastic shock wave are discussed in terms of specific features of the multiplication kinetics. In our experiments with shockless compression we have revealed an apparent reverse dependence of recorded Hugoniot elastic limit upon the compression rate which is explained by wave interactions at the reflection of elastic-plastic compression wave from the sample surface. A manifestation of stress relaxation at shock compression of hard ceramics and glasses is also discussed. Financial support from the Russian Science Foundation via grant No. 14-12-01127 is gratefully acknowledged.

One- and two-stage cumulative Mach-type shock wave generators

Nikolaev D N[@], Kvitov S V, Shutov A V and Ternovoi V Ya

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] nik@ficp.ac.ru

The main goal of presented work was the need to increase the size of shock wave, in comparison with 16 mm described in [1], for the purpose of experimental investigation of dynamic compression of gases. Devices with high explosive (HE) mass 13 kg with fully cylindrical geometry are proposed. Imploding conical detonation wave (DW) in cylindrical HE charge with demanded cone angle is forced by controlled sequential initiation of charge along its side cylinder surface by detonation distributor. Detonation products is used to launch the copper liner toward the axis of device, dynamically forming the conical shape of liner. Its impact with the cylindrical central body—brass tube with polymethylmethacrylate (PMMA) filling—drives the imploded conical shock wave in PMMA, leads to formation of Mach configuration and the origin of flat Mach disk. One-stage device provides shock wave in PMMA with diameter of 20 mm and velocity up to 20 km/s, and generates pressure up to 0.6 TPa in iron sample. To increase the parameters of device, the two-stage generator was developed. The second stage liner, consisted of copper tube, covered with HE layer, was introduced to increase the liner velocity before impact. Together with decrease of the diameter of central body up to 10 mm and with adjusted geometry of conical DW in main HE charge, this led to increase of velocity of mach disk up to 30 km/s, allowing to reach 2 TPa in iron. The issues of influence of geometry of conical DW on the growth of mach disk and the results of numerical 2-D hydrodynamic simulation of experimental devices with various geometry will be discussed, along with the first results on Hugoniot measurements.

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Energy dissipation rate in copper subjected to the high pressure loading

Borodin E N[1,3,2,@], Mayer A E[2], Podurets A M[4], Beluhina P S[4], Grebennikova S E[4], Tkachenko M I[4] and Balandina A N[4]

[1] Institute of Problems of Mechanical Engineering of the Russian Academy of Sciences, V.O., Bolshoj pr., 61, Saint Petersburg 199178, Russia
[2] Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia
[3] Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia
[4] Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia

[@] elbor7@gmail.com

We have performed numerical calculations and microstructure investigations of the defect structures and energy dissipation rate due to the shock wave propagation in copper with different pressure amplitudes, from 2 to 150 GPa. Various aspects of plasticity such as the role of the equation of state, the strain hardening, the energy dissipation rate are investigated on the basis of the structural models for dislocation plasticity and mechanical twinning. Calculations revealed that from the structural point of view the material response on the external loading is considerably different in the case of weak shock wave loading with pressure amplitude about several Gigapascals from its response on loading by shock waves with pressure amplitude above 20 GPa. In order to verify our results, we also compare them with new original experimental data of the differential scanning calorimetry. We discuss the fraction of the plastic dissipation work, which is stored in the defect structure of material at various amplitude of external loading.
This study was supported by grants of the Russian Foundation for Basic Research (project No. 16-31-60051) and the Ministry of Education and Science of the Russian Federation (competitive part of State Task of NIR CSU No. 3.1334.2014/K).

Investigation of the magnesium alloy AZ31 before and after the accumulative roll-bonding under high strain rate

Garkushin G V[1,2,@], Razorenov S V[1,2], Kruger L[3] and Lange K[2]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] Tomsk State University, Lenina Avenue 36, Tomsk 634050, Russia

[3] Institute of Materials Engineering, Technical University Bergakademie Freiberg, Gustav-Zeuner-Straße 5, Freiberg D-09596, Germany

[@] garkushin@ficp.ac.ru

Accumulative roll-bonding (ARB) is one of the promising directions in the field of bulk large metal bars with fine-grained structure. In this case, the study of the similar materials over the wide range of stain rate 10^{-5} to 10^{5} s^{-1} to identify the mechanisms of deformation and fracture and their correlation with the internal microstructure is of interest. The processes of high strain rate and fracture caused by the shock wave in such materials have not been studied. In this work the samples were studied magnesium alloy AZ31 before and after the accumulative roll-bonding. The alloy density is 1.77 g/cm^3. Structural data were obtained by optical microscopy. As-received samples before treatment had the uniform structure with a grain size of 21 μm. Modification of magnesium alloy samples using ARB has reduced the grain size to 4 μm. The samples were annealed at 400°C for 24 hours after rolling. The plane shock waves in the samples were generated by impacts of aluminum plates 2 and 0.45 mm in thickness accelerated with explosion to a velocity of 630 ± 30 m/s. Varying the thickness of the impactor allowed to change the strain rate under fracture of magnesium alloy samples. The free surface velocity histories were monitored with the VISAR. The obtained values of the Hugoniot elastic limit and the dynamic strength in the as-received samples and after ARB virtually are unchanged.

Surface fracture energy of pulse action

Krivosheev S I[@] and Magazinov S G

Peter the Great Saint-Petersburg Polytechnic University, Polytechnicheskaya 29, Saint-Petersburg 195251, Russia

[@] ksi.mgd@gmail.com

The destruction of materials at pulse impact is carried out using a limited set of loading schemes. The magnetic pulse method allows studying material properties in samples with macro defects of mode of cracks. One of the main features of this method is the possibility to create controlled pressure pulses in the microsecond duration range with amplitude up to 2 GPa. The detailed technique is described in [1]. The stress state of all samples was analyzed using ANSYS simulation software. Simulation results correspond to the shock-wave loading mode. The criterion, which allows identifying the material parameter (energy accumulation time) for determining the formation of start conditions for the fracture, was formulated on the basis of the thermodynamic approach [2]. The applicability of this criterion for describing the fracture of samples upon spallation loading scheme and samples with macro defects of mode of cracks was shown. The growth of starting surface energy with increasing load was revealed. The scale of the critical areas for energy accumulation was determined and the relation between the surface fracture energy and the material parameter, such as the energy accumulation time required for fracture, was revealed.

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The metal rings fracture under expansion by magnetic pulse method of microsecond duration

Atroshenko S A

Institute of Problems of Mechanical Engineering of the Russian Academy of Sciences, V.O., Bolshoj pr., 61, Saint Petersburg 199178, Russia

satroshe@mail.ru

Study of copper and aluminum ring samples was performed on magnetic pulse installation. It was used two developed by V A Morozov [1] loading techniques based on a high pulse current generator, which reduced the period of the harmonic load of up to 100 ns. The study of the fracture surfaces of aluminum revealed almost viscous character of destruction at long loading pulses. In the case of short pulses the quantity of fibers in the fracture surface is reduced and cracks are observed, and also twins appear, which is surprising for a material with high stacking fault energy. Also in the case of a short-pulse loading dynamic recrystallization occurs with the emergence of new small grains. Dynamic recrystallization is observed in the copper samples after loading, as well as the shear band.

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Characterization of residual stress-strain state after the steel and titanium cylinders explosive coupling

Ananev S Yu, Borodina T I, Val'yano G E, Deribas A A and Yankovsky B D[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] yiy2004@mail.ru

Conducted the crimping of cylindrical parts made of stainless steel and titanium by radially converging detonation wave. As a result of crimping has occurred a coupling of cylinders through the plastic deformation of structural parts. The copling was followed by a reduction of the external steel cylinder thickness (10%) at its simultaneous lengthening. The x-ray diffraction analysis showed that explosive loading of titanium-steel cylinders pair led to transition of a steel condition from single-phase austenic to the two-phase (ferritic-austenic). The content of ferrite in the different areas of a detail fluctuates from 56 to 100% vol. depending on loading value. It is known that such transition is followed by volume increase on 4.57%. The parameter of austenite crystal lattice into all studied sites exceeds the parameter of initial steel lattice. In addition, impact loading led to increasing in deformation of an austenite crystal lattice. Growth of lattice micro distortions to 1.3–2.7 times in comparison with initial level is observed. The changes into titanium, caused by crimping of cylinders, are expressed more weakly than into steel. There is a compression of an elementary cell of titanium crystal lattice for 1.4% in comparison with initial material. Optical surface analysis of the etched samples showed changes in the shape of a grain titanium structure and the characteristic size of the grains within the deformation detail defects. In the area of intensive titanium deformation the group of grains elongated along the plastic shear, and the characteristic size decreased from 20 μm inside the body part to $\sim$ 2 μm in the boundary layer. The structure of stainless steel samples has significantly smaller changes.

Numerical simulation of wave formation mechanism in explosive welding

Sultanov V G[@] and Shutov A V

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] sultan@ficp.ac.ru

In the work, the results of the direct numerical simulation of wave formation in explosive welding are presented. The elastic-plastic model of media motion [1], wide-range equations of state for metals [2], the equation of state of explosives, explosion products and kinetics of decomposition of explosive substances [3] were used in two-dimensional numerical simulations.
Effect of different boundary conditions (no-slip and full slip) between plates on the nature of the wave formation was investigated.
It was shown that in case of no-slip condition the wave formation is described by Kudinov–Koroteev mechanism [4]. In the case of full slip, the wave formation mechanism is similar to the Kudinov–Koroteev mechanism, but has a number of features.

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The study of the defect structures evolution in metals during the gigacyclic fatigue test

Vshivkov A N[@], Prokhorov A E and Plekhov O A

Institute of Continuous Media Mechanics of the Ural Branch of the Russian Academy of Sciences, Academician Korolev Street 1, Perm 614013, Russia

[@] vshivkov.a@icmm.ru

In this paper, the defect structures evolution of metals are studied experimentally [1]. The ultrasonic testing machine USF-2000 was used to carry out fatigue tests involving $10^6 - 10^{10}$ loading cycles. The frequency of loading is 19.5 ± 0.5 kHz [2]. Based on the experimental data, the Whler curve was obtained. For the analysis of physical condition, the sensor was designed, which measure the electric potential drop of the sample. This measuring method can be applied to conductive materials such as metals. It was shown that the significant changes in physical processes accompanying the evolution of structural defects in the material were observed in the final stages of the experiment. The applied measurement technique allows us to exactly determine the time of fatigue crack initiation below the surface of the sample, which cannot be monitored by standard optic methods.

The work was supported by the projects of RFBR No. 16-31-00155 and No. 16-31-00130.

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Experimental study of mechanical properties of liquids under shock wave loading

Bannikova I A[1,@], Uvarov S V[1], Zubareva A N[2], Utkin A V[2] and Naimark O B[1]

[1] Institute of Continuous Media Mechanics of the Ural Branch of the Russian Academy of Sciences, Academician Korolev Street 1, Perm 614013, Russia
[2] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] malgacheva@icmm.ru

Experiments on shock wave loading of liquids (glycerol, silicone oil and transformer oil) with different layer thicknesses to determine the relaxation and strength properties were carried out. Shock wave loading was realized by using explosives [1]. Free surface velocity profiles were measured by system VISAR. Types of velocity profiles obtained in glycerol were different from the velocity profiles obtained in transformer oils and silicone oils. The power laws of stress amplitude and spall strength on the strain rate were found for the compression fronts (range from 10^5 to 10^7 s^{-1}) and rarefaction fronts (range from 10^4 to 10^5 s^{-1}). Spall strength of oils proved a constant and weakly depends on the strain rate and temperature. The power laws reflect the self-similarity nature of the mechanisms of momentum transfer [2] and failure of liquid [3] that are observed traditionally in solid [4] due to the mechanisms of defect induced structural relaxation [5].

This work was supported by grants RFBR No. 16-31-00283, 14-01-96012, 14-01-00842.

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Study of explosive loading of natural materials

Orlov M Yu[@], Orlova Yu N and Bogomolov G N

Research Institute of Applied Mathematics and Mechanics of the Tomsk State University, Lenin Avenue 36, Tomsk 634050, Russia

[@] orloff_m@mail.ru

At the present time investigation of the behavior of natural materials under explosive loading are relevant. This is due to the development of the northern territories, the extraction of natural resources in the Far North, etc. The objects of study were the river ice and natural limestone. The practical significance of research due to the need to increase production of oil and gas in permafrost regions, the fight against ice jams, etc. Three years ago, it was organized by a scientific mobile laboratory "Explosive destruction of the natural materials" at the National Research Tomsk State University. The main purpose of the laboratory is express analyzing of explosive destruction of natural materials, including ice, limestone, granite, coal, etc.

It was made full-scale experiments to undermine the snow-covered ice, bar ice, sandwich ice and natural limestone. The experimental results can be used only as a qualitative test for the numerical simulation. In this paper has conducted a few full-scale experiments. The first experiment was undermining river of ice of emulsion explosives in water. The second experiments was undermining limestone of various explosives (three types of explosives). It was found a video of the experiment, the diameter of the blast lane and the crater, estimated radius of debris cloud.

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The role of decompression and micro-jetting in shock wave synthesis experiments

Schlothauer T[1,@], Schimpf C[2], Kroke E[1], Heide G[3] and Schwarz M R[1]

[1] Institute of Inorganic Chemsitry, Technical University Bergakademie Freiberg, Leipziger Strasse 29, Freiberg D-09596, Germany
[2] Institute of Materials Science, Technical University Bergakademie Freiberg, Gustav-Zeuner-Strasse 5, Freiberg D-09596, Germany
[3] Institute of Mineralogy, Technical University Bergakademie Freiberg, Brennhausgasse 14, Freiberg D-09596, Germany

[@] schlotha@mineral.tu-freiberg.de

Despite the fact that the use of powders of copper and other metals as impedance medium for high pressure shock wave synthesis of diamond was developed in the 1960ies [1] and is still an important ingredient in the shock synthesis of refractory materials today [2], the processes in the metal powder itself are still not well understood. For this reason the behavior of the impedance powder was investigated at conditions and capsule geometries comparable with those previously used for the succesful shock synthesis of the high pressure form of silicon nitride [3]. Our planar impact experiments with copper powders compressed to comparable initial densities revealed a great sensitivity of the microjetting processes on the degree of free intergranular spaces. With hindsight it is found that the yield of recovered high pressure phase was highest for those synthesis runs with intense jetting. This improves the comparability between experiments, but reduces simultaneously the output on HP-phase.

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Chemical composition and shock compression of basalt from the vicinity of a natural meteorite crater

Nikolaev A Yu[@], Kozlov E A, Yusupov D T, Sidorov K S, Klenov A I, Petukhov E A, Yurchenko O S, Smachnaya O V, Lysenko O V and Sedova O V

Federal State Unitary Enterprise "Russian Federal Nuclear Center—Academician Zababakhin All-Russian Research Institute of Technical Physics", Vasilieva 13, Snezhinsk, Chelyabinsk Region 456770, Russia

[@] AlexeyRX350@yandex.ru

This presentation gives data on chemical composition, average density of the four basalt samples that were taken from the vicinity of a natural meteorite crater. It also shows the set-ups of explosive experiments and the first results on shock compression for the rock in weak and strong shock waves with amplitudes of 7.6–80 GPa. The obtained results will be used for numerical modeling of the wave processes in recovered samples of the same rock that were subjected to low- and high-intensity explosive loading.

Structural transformations and amorphization of silica modifications under shock wave loading

Zhukov A N[1,@], Yakushev V V[1], Galkin R S[1,2] and Rogacheva A I[1]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] Lomonosov Moscow State University, Leninskiye Gory 1, Moscow 119991, Russia

[@] azhukov@icp.ac.ru

Three silica polymorphs: quartz, cristobalite, and tridymite were shock wave loaded by high temperature shock compression method similar that used in [1]. According to the method the samples put in copper recovery ampoules were shock compressed using planar loading scheme. Shock waves were generated by aluminum plates accelerated with detonation products of various explosives to several km/s. Depending on using explosive and experimental setup pressure in samples were 14, 22, 28, 33, 37, and 50 GPa. After shock wave experiment and recovering from the ampoule the samples were purified with boiling acids. Then the samples were investigated by the x-ray powder diffraction method. Diffraction patterns give evidence that quartz, cristobalite, and tridymite at shock compression to 14–28 GPa undergo some structural transformation with partial amorphization, under higher pressure all three modifications of silica amorphize almost completely. Structural transformation of quartz is arisen from generation of crystal structure faults. Structural transformation of cristobalite and probably tridymite is most likely phase transformation without changing coordination number or radical crystal structure reconstruction.

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Morphological turning, electroconductivity and structural phase transitions of shocked titanium

Golyshev A A[1,@], Kolobova A Yu[2], Kudymova Yu E[1] and Molodets A M[1]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] Institute of Structural Macrokinetics and Materials Science of the Russian Academy of Sciences, Academician Osipyan 8, Chernogolovka, Moscow Region 142432, Russia

[@] golyshev@icp.ac.ru

Coarse-grained Ti (c-Ti) and nanocrystalline titanium (nc-Ti) metal was investigated up to 120 GPa using a flyer plate impact technique. The metal flyer velocity was in the range of 2–3 km/s, and the shock pressure was calculated to be 40–120 GPa. Electrical resistance techniques were used to investigate the structural phase stability of titanium in-situ. A shock recovery experiment for c-Ti and nc-Ti was performed by a flyer plate impact technique. The shock-treated samples were characterized by x-ray diffraction analysis, optical microscopy and transmission electron microscopy.

The grain size of c-Ti is observed to undergo twenty-fold reduction. The high-pressure experiments on nc-Ti samples do no show the significant variation of the grain sizes. The electrical resistance of c-Ti and nc-Ti samples has been measured under conditions of step shock compression and following release wave. The history of shockwave loading of titanium has been calculated using the semiempirical equations of state. It has been shown that in the phase of compression at a pressure of $\sim$ 80 GPa, the resistance of nc-Ti titanium samples stepwise reversible changes just as for c-Ti. The observed effect is interpreted as a consequence of the polymorphic transition in shocked nc-Ti as well as for c-Ti earlier [1].

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Physicochemical transformation and equations of state of boron over megabar shock pressure

Molodets A M[@], Golyshev A A and Shakhray D V

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] molodets@icp.ac.ru

A shock recovery experiment for amorphous and crystalline boron powder was performed by a flyer plate impact technique. The metal flyer velocity was in the range of 2–3 km/s, and the shock pressure was calculated to be 40–120 GPa. The calculations were performed by the hydrocode with user created semiempirical equation of state for amorphous and crystalline boron. The shock temperature and specific volume of shocked boron was calculated also. The shock-treated samples were characterized by x-ray diffraction analysis, and studied by measuring the dynamic magnetic susceptibility. No changes of amorphous boron or unknown compounds are observed up to shock pressure 40 GPa. X-ray diffraction analysis reveals the presence of new structures in the recovered samples in shock pressure 50–120 GPa. One of possible version is the transformation of elemental boron. The origination of reaction products between the contacting ampoule metals and boron powder particle were also discussed. The shock wave induces a physicochemical transformation not only in amorphous boron but also in crystalline boron.

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Electrical conductivity of amorphous boron under shock wave compression

Shakhray D V[@], Golyshev A A and Molodets A M

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] shakhray@icp.ac.ru

Elementary boron is important material of nuclear power. Boron exists in a crystalline and amorphous state. The phase diagram of crystal boron has difficult structure, in the high pressures and temperatures area deficiency of experimental and settlement information on thermophysical properties is noted. As for amorphous boron, experimental data about its thermohysical properties at high pressures are limited. The reached parameters of pressure and temperature of the sample allow to capture considerable area of the boron phase diagram including area of high pressures and temperatures (up to 150 GPa and 2000 K) with possibility of purposeful change of a phase trajectory. In this work, experiments on shock wave loading of samples of amorphous boron up to the pressure 100 GPa with simultaneous measurement of conductivity are made. Samples represented a flat disk with a diameter of 10 mm and 1 mm thick. It is shown that with a pressure up to 15 GPa it is not found any changes on dependence of resistance on pressure. However with pressure over 15 GPa sharp reduction of resistance to 1 Ohm is recorded. By means of the developed equation of state values of temperature and density of boron under compression are calculated. Samples of shocked amorphous boron subjected shock wave compression was investigated by methods of x-ray diffraction for detection of possible allotropic transformations of amorphous boron in shock waves.
This work was supported by Rosatom contract H.4x.44.90.13.1112

Thermodynamic properties and electrical conductivity of expanded copper

Emelyanov A N[@] and Shakhray D V

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] emelyanov@ficp.ac.ru

Under certain conditions, metal-nonmetal transition occurs in the expanded metals near critical point [1]. The critical point parameters of metals cannot be analyzed without considering their relation to the metal–nonmetal transition. The transition metal-nonmetal was studied for a limited number of metals. They are cesium, rubidium and mercury [2]. There are only theoretical works [3,4], and limited number of works on the electrical explosion of metallic wires and foils [5,6] for other metals. Study of thermodynamic parameters of copper in near-critical point region of liquid-vapor phase transition and the predicted metal–nonmetal transition was carried out. The measurements of electrical conductivity of copper after shock compression and expansion in gas (helium) medium at different final pressure were carried out. The electrical conductivity of expended copper is 10^4–10^6 times lower than the electrical conductivity of copper under normal conditions. It was discovered, registration of time dependence of electrical resistivity of the expanded metal provides of estimating their density in the near-critical point region of liquid–vapor phase transition.

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Synthesis of superconducting compounds on the basis of Al and Al_2O_3

Avdonin V V[1,@], Shakhray D V[1] and Palnichenko A V[2]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] Institute of Solid State Physics of the Russian Academy of Sciences, Institutskaya Street 2, Chernogolovka, Moscow Region 142432, Russia

[@] avdonin@icp.ac.ru

It is known that granular films of some superconductors exhibit enhancement of the superconducting transition temperature T_c, compared to that in the bulk, when the grain size is small enough. For example, in aluminum [1] this effect is about a double value of $T_c = 1.2$ K for the bulk. Moreover, it has been found that the films with comparable grain size evaporated at low temperatures in oxygen-free ambience [1] and at room temperature in oxygen atmosphere demonstrate similar enhancement of the T_c, which led to a conclusion that the aluminum oxide itself does not participate in the T_c-enhancement mechanism. The only role of oxygen has been considered to conserve small aluminium grains with aluminium oxide coating, thus stabilizing the fine-grain structure of the Al films, which results in stabilization of the enhanced T_c [2]. In this work, a mixture of Al and Al_2O_3 has been subjected to a shock-wave pressure of 170 kbar, followed by vacuum-encapsulating and quenching of the product to liquid nitrogen. The *ac* magnetic susceptibility measurements of the samples have revealed metastable superconductivity with $T_c = 37$ K.

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Activities on proton radiography at the Institute for Theoretical and Experimental Physics

Golubev A A[@] and Kantsyrev A V

State Scientific Center of the Russian Federation "Institute for Theoretical and Experimental Physics", National Research Center "Kurchatov Institute", Bolshaya Cheremushkinskaya 25, Moscow 117218, Russia

[@] golubev@itep.ru

The first activity on proton beam application to radiography was started about 45 years ago. Existing proton radiography facilities in USA (pRad in LANL), Russia (PUMA in ITEP) and Germany (prototype of PRIOR in GSI) clearly demonstrated the advantages of the high-energy proton radiography method with magnetic optics compared to conventional x-ray techniques in the study of solid objects and dense plasma, especially in dynamic experiments. Jointly constructed, by teams of scientists from GSI, ITEP, IPCP and LANL, proton radiogrpahy setup PRIOR (proton microscope for FAIR) was commissioning in 2014. In the first experiments at PRIOR with 3.6 GeV proton beam from SIS-18 accelerator at GSI a spatial resolution of 30 μm was achieved. The new project of 247 MeV proton microscope is being developed by ITEP, INR and IPCP's team. Such setup is designed for investigation of density distribution for static objects and shock-wave processes in dynamic objects with areal density of up to 5 g/cm^2. Developed project allows investigation the phenomenon of anomalous compressibility for porous rubber and docosane, compessibility of non-ideal plasma of Xe and Ar gases under shock wave loading. Proton beam with energy of 247 MeV is available at high-current linear accelerator of Moscow Meson Factory (MMF) in INR Troitsk, Russia. MMF accelerator designed to operate at frequencies up to 100 Hz, which will additionally explore the slow-changing dynamic processes such as crystallization and melting. The calculation of ion-optical scheme of setup and Monte-Carlo modeling at GEANT for static object were performed.

Reconstruction of targets volume density in proton radiography experiments

Kolesnikov D S[1,2,@], Kantsyrev A V[1,2], Golubev A A[1,2] and Varentsov D V[3]

[1] State Scientific Center of the Russian Federation "Institute for Theoretical and Experimental Physics", National Research Center "Kurchatov Institute", Bolshaya Cheremushkinskaya 25, Moscow 117218, Russia
[2] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[3] GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, Darmstadt 64291, Germany

[@] dstorm1@mail.ru

Series of experimental investigation of extreme states of matter generated by shock–waves were performed at proton microscopy facilities PUMA [1] at ITEP and PRIOR [2] at GSI. Reconstruction of targets volume density from radiography images (areal density distributions images) is important task at such experiments.
To solve the problem of reconstruction of volume density the recurrence algorithm of inverse Abel transform [3] was implemented in Matlab. During the tests it was revealed that the algorithm is very sensitive to noise in the original data. Application of the multilevel tresholding algorithm [4] has increased the range of acceptable noise ratio from 4 to 30%. Deconvolution method based on Lucy–Richardson algorithm was implemented to compensate blur of images. Demonstarion of developed tools was performed with results of underwater electrical wire explosion experimente at PRIOR facility at GSI and investigation of detonation of TNT at PUMA facility at ITEP.

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Numerical simulation of 247 MeV proton microscope

Bogdanov A V[@], Kantsyrev A V, Golubev A A, Demidova E V, Kolesnikov D S, Panyushkin V A, Markov N V and Vysotsky S A

State Scientific Center of the Russian Federation "Institute for Theoretical and Experimental Physics", National Research Center "Kurchatov Institute", Bolshaya Cheremushkinskaya 25, Moscow 117218, Russia

[@] toshka87@list.ru

High-energy proton radiography is widely uses for investigation of the internal structure of dense static and dynamic objects. The advantage of the proton-radiographic studies in comparison with usual x-ray radiography is a better penetrating power, better dynamic range and spatial resolution. Most impressive results in this field were obtained on experimental setups, which operate on a proton microscope scheme. At the meson facility of the Institute for Nuclear Research (Troitsk), it is possible to create a proton-radiographic setup operating on the energy of 247 MeV. The feature of this project is the possibility to use the equipment previously used for creating PUMA facility (ITEP, Moscow) [1]. Program for the simulation was created with COSY Infinity code [2]. This program is providing optimization of parameters of setup such as field of view, magnetic fields, the relative position of the magnetic elements and quality of proton radiographic image. In addition, calculations were verified by Monte Carlo method with GEANT simulation of experiments with static objects. At new setup is planned to investigate of the phenomenon of anomalous compressibility of porous rubber and docosane [3], compressibility of nonideal plasma of Xe and Ar gases under shock-wave loading.

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Shock wave compression of carbon fiber

Mochalova V M[1,2,@] and Utkin A V[1,2]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] Tomsk State University, Lenina Avenue 36, Tomsk 634050, Russia

[@] roxete20000@hotmail.com

Carbon fibers are composite materials, which consist of fibers from carbon with a diameter of 5–10 microns bonded with epoxy resin. Main feature of these materials is strongly expressed anisotropy of properties. The aim of this work is to investigate the shock compressibility of carbon fiber with different fibers orientation relatively to the direction of shock waves propagation. The average density of the samples was 1.55 g/cm^3. The sound speed transversally to the fibers is equal to 3.0 km/s, and parallel is about 10 km/s. Shock wave profiles were registered by a laser interferometer VISAR. In each experiment the structure of compression pulse and the shock wave velocity of carbon fiber were obtained. Pressure of shock compression was varied by changing of the thickness and the velocity of projectiles. From the experiments Hugoniots of carbon fiber were obtained for parallel and transverse orientation of the fibers in the coordinates of the shock wave velocity D—particle velocity u. In the investigated range of pressures at the transverse orientation of the fibers experimental data are satisfactorily approximated by a linear dependence of $D = 1.70 + 2.3u$, km/s. The Hugoniot for the parallel orientation is satisfactorily approximated by the dependence $D = 2.3 + 2.0u$, km/s. Unlike the transverse orientation, in this case a complex structure of the shock wave is observed—almost in the entire pressure range two-wave configuration is recorded which is most clearly expressed at low pressures. The velocity of propagation of disturbances along the carbon fibers is in several times higher than the velocity of the shock wave, that results in the formation of a precursor. The work is carried out with the financial support of FAIR-Russia Research Center.

Experimental study of dynamic properties of porous materials under shock-wave loading

Zubareva A N[1,2,@], Efremov V P[3] and Utkin A V[1]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] State Scientific Center of the Russian Federation "Institute for Theoretical and Experimental Physics", National Research Center "Kurchatov Institute", Bolshaya Cheremushkinskaya 25, Moscow 117218, Russia

[3] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] zan@ficp.ac.ru

New experimental data on the properties of porous materials under shock-wave loading and spallation strength were obtained for samples prepared from matrix materials with different compressibility: silicone rubber and epoxy resin. Porosity in samples was set up by using glass microspheres with an average size of about 80 microns as a filler. Free surface velocity profiles of samples under shock-wave loading were registered with VISAR. Obtained velocity profiles had a rather complex structure of the shock-wave front. A possible reason for that is the kinetics of pore collapse in studied heterogeneous samples. Silicone rubber with microspheres showed itself as a material with the low value of damage threshold. Its calculated spall strength is 15 MPa. The wave structure of epoxy resin with microspheres obtained in the experiments is qualitatively similar to the results observed with rubber as a matrix material. Quantitative difference between them is due to the difference between shock-wave properties of the matrices. In particular, the disappearance of the first wave for rubber occurs at a pressure of about 1 GPa, which is significantly earlier than for epoxy resin at a pressure of about 2 GPa. Hugoniots of studied samples were obtained by processing the experimental results.

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Two-stage light-gas magnetoplasma accelerator for hypervelocity impact simulation

Khramtsov P P, Vasetskij V A, Makhnach A I[@], Hryshchanka U M, Chernik M Yu, Shikh I A and Doroshko M V

Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus, P Brovka Street 15, Minsk 220072, Belarus

[@] mahnach_anna@mail.ru

The development of macroparticles acceleration methods for high-speed impact simulation in a laboratory is an actual problem due to increasing of space flights duration and necessity of providing adequate spacecraft protection against micrometeoroid and space debris impacts. This paper presents results of experimental study of a two-stage light-gas magnetoplasma launcher for acceleration of a macroparticle, in which a coaxial plasma accelerator creates a shock wave in a high-pressure channel filled with light gas. Graphite and steel spheres with diameter of 2.5–4 mm were used as a projectile and were accelerated to the speed of 0.8–4.8 km/s. A launching of particle occurred in vacuum. For projectile velocity control the speed measuring method was developed. The error of this metod does not exceed 5%. The process of projectile flight from the barrel and the process of a particle collision with a target were registered by use of high-speed camera. The results of projectile collision with elements of meteoroid shielding are presented. In order to increase the projectile velocity, the high-pressure channel should be filled with hydrogen. However, we used helium in our experiments for safety reasons. Therefore, we can expect that the range of mass and velocity of the accelerated particles can be extended by use of hydrogen as an accelerating gas.

Optical diagnostics of laser-generated shock waves at LUCH laser facility

Kuznetsov A P[1,@], Gubskii K L[1], Derkach V N[2], Belkov S A[2], Garanin S G[2] and Golovkin S Yu[2]

[1] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[2] Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia

[@] apkuznetsov@mephi.ru

Equation-of-state experimental tasks of the LUCH laser facility and role of optical diagnostics are described. Current state of the optical diagnostic system and objectives of the ongoing modernization is discussed. The modernization includes constructing of active interferometric technique for measuring of shock velocity based on line-imaging velocimeter type in addition to passive SOP method.

Interferometers for measuring velocity in shock-physics experiments

Gubskii K L[@], Mikhaylyuk A V, Koshkin D S, Norkin S V and Kuznetsov A P

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

[@] kgubskiy@mail.ru

Studying extreme states of matter exposed to intense pulsed loads is rather complicated due to a number of setup features of the experiment. The uniqueness of experiments and inability to repeat them under identical conditions place heavy demands on output data. An important scientific problem in the physics of extreme states of matter, which is of great practical importance, is the study of physical and mechanical properties of materials exposed to intense dynamic loads, produced by powerful explosion shock waves, hypervelocity impact or laser pulse. Most informative contactless method in such experiments is Doppler interferometry, that allows to carry out continuous surface velocity measurement.The description and analysis of the possibilities of the main types of interferometric velocity measuring devices used in physics, physics of shock waves and extreme states of matter at the present time—PDV, VISAR, ORVIS, Line-imaging velocimeter, etc. presented.

Laser diagnostic system for velocity measuring in high energy physics experiments

Mikhaylyuk A V[@], Koshkin D S, Gubskii K L and Kuznetsov A P

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

[@] andrey1990_mephi@mail.ru

The paper presents the diagnostic system for velocity measurements of reflecting objects. The system is designed to measure speed in the interval of 5 to 50 km/s. Powerful laser pulses expose the target and generate shock waves inside it. The back side of target is illuminated by probe laser beam at a wavelength of 660 nm. The diffused and reflected probe light is collected by a lens and injected into the optical system. Two Mach–Zehnder interferometers with different reference delay etalons form a vernier measuring system. Also, the system includes a passive channel that records glow luminescence in the shock wave front. The spatial resolution of the measuring system on the target is about 4 μm.

Vernier VISAR interferometer system for measuring shock wave velocity

Koshkin D S[1,@], Mikhaylyuk A V[1], Gubskii K L[1], Antonov A S[2] and Kuznetsov A P[1]

[1] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[2] Limited Liability Company "Laser Eye", Kashirskoe Shosse 31, Moscow 115409, Russia

[@] koshkin.dimitri@gmail.com

An important scientific problem in high-energy-density physics is the study of the physical and mechanical properties of materials exposed to intense dynamic loads. The uniqueness and complexity of experiments place heavy demands on research methods. Doppler interferometry is the most widespread contactless method that allows to carry out continuous surface velocity measurement. Quadrature-differential VISAR systems are reliable and relatively inexpensive devices providing sufficient accuracy and time resolution for most experiments. Standard quadrature-differential interferometers are designed for simultaneous measurement of the velocity of only one point on an object. Moreover, due to limitations of photoregistration device "missing" of interference periods can occur when observing steep shock front.

To overcome this limitations vernier VISAR diagnostic system was designed. This system is combination of optical and electronic units interconnected by optical fibers. Two quadrature-differential VISAR interferometer form a vernier system, that allows to obtain exact parameters of shock front regardless of interference periods "missing". Each optical unit designed to produce independent analysis of up to 7 optical channels. Changeable delay etalons with different optical path length allows to extend systems dynamic range. The basic operations with the interferometer may be performed remotely from a personal computer using special software.

A numerical method for calculating interior ballistics of electrothermal accelerator

Vorobiev A A

Military Academy of Strategic Rocket Troops after Peter the Great, Kitaygorodskiy 9, Moscow 109074, Russia

vorobievall@mail.ru

Electrothermal accelerator (ETA) uses high-voltage arc energy to heat the actuating medium, it being made from low-molecular weight material. Projectile acceleration is achieved by expansion of the actuating medium. ETA structure, operating principle and some results are presented in [1, 2]. Numerical method for calculating interior ballistics uses Lagrangian coordinates there the conservation of momentum is solved. A statement of the energy balance in differential form reflects the second law of thermodynamics:

$$\frac{\partial \mathrm{E}}{\partial t} = -\left(P + Q\right)\frac{\partial V}{\partial t} + B\left(t\right).$$

The B-term symbolizes an energy input rate. In the case of ETA B-case term is the energy of high-voltage arc in the discharge chamber. Lagrangian different grid and scheme for numerical calculation were used as in [3]. Fully explicit scheme was employed. The solving includes two stability conditions: Courant and shock (artificial viscosity Q). Numerical results were compared with the experimental research for pressure in the ETA barrel. The research was conducted under financial support of the Ministry of Education and Science of Russia within the Russian President grant No. MK-5250.2016.8.

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Simulation of systems for shock wave/compression waves damping in technological plants

Sumskoi S I[1,@], Sverchkov A M[2], Lisanov M V[2] and Egorov A F[3]

[1] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[2] Scientific and Technical Centre "Industrial Safety Research", Perevedenovsky 13 Bldg 14, Moscow 105082, Russia
[3] Mendeleev University of Chemical Technology of Russia, Miusskaya Square 9, Moscow 125047, Russia

[@] sumskoi@mail.ru

At work of pipeline systems, flow velocity decrease can take place in the pipeline as a result of the pumps stop, the valves shutdown. As a result, compression waves appear in the pipeline systems. These waves can propagate in the pipeline system, leading to its destruction. This phenomenon is called water hammer (water hammer flow).
The most dangerous situations occur when the flow is stopped quickly. Such urgent flow cutoff often takes place in an emergency situation when liquid hydrocarbons are being loaded into sea tankers. To prevent environment pollution it is necessary to stop the hydrocarbon loading urgently. The flow in this case is cut off within few seconds.
To prevent an increase in pressure in a pipeline system during water hammer flow, special protective systems (pressure relief systems) are installed.
The approaches to systems of protection against water hammer (pressure relief systems) modeling are described in this paper. A model of certain pressure relief system is considered. It is shown that in case of an increase in the intensity of hydrocarbons loading at a sea tanker, presence of the pressure relief system allows to organize safe mode of loading.

Simulation of compression waves/shock waves in the branched pipeline systems

Sumskoi S I[1,@], Lisanov M V[2], Sverchkov A M[2,3] and Egorov A F[3]

[1] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[2] Scientific and Technical Centre "Industrial Safety Research", Perevedenovsky 13 Bldg 14, Moscow 105082, Russia
[3] Mendeleev University of Chemical Technology of Russia, Miusskaya Square 9, Moscow 125047, Russia

[@] sumskoi@mail.ru

Shock waves/compression waves (SW/CW) can have a negative impact. Typically, the SW/CW attenuate during their propagation. However, in practice, there are flows that are nearly one dimensional, and there is not significant attenuation of SW/CW in such flows. In this case, SW/CW can propagate over long distances (up to tens of kilometers), maintaining its damage potential.
The most well-known example of weakly attenuated SW/CW propagation is water hammer flow in pipeline systems. This task can be set and resolved quite accurately in one-dimensional formulation, and multidimensional effects, if any take place, are taken into account as well.
This article presents a mathematical model and a numerical method for solving the problem of water hammer flow in the branching pipe. The problem is considered in the one-dimensional non-stationary formulation including changing diameter of the pipeline and its branches.
We have solved the problem of CW propagation in the complex branching pipeline system. It was shown that in case of water hammer flow the highest pressures in branches of the pipeline can be achieved when asynchronous valve shut-down takes place, while in previous studies only simultaneous shut down was considered.

Numerical investigation of the behavior of the composite rarefaction wave in hot nuclear matter in the presence of entropy perturbations

Konyukhov A V[@] and Likhachev A P

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] konyukhov_av@mail.ru

The interaction of the composite rarefaction wave in nuclear matter with entropy nonuniformities is studied numerically. Gasdynamic nonuniformities in an expanding fireball of the quark-gluon plasma resulting from the secondary interaction of reaction products with nucleons of colliding nuclei are assigned in calculations as initial conditions: inside the fireball the pressure is supposed to be uniform, the distribution of the baryon number density is given by $n = n_0(1+\alpha \sin(kx) \sin(ky))$. The fireball expansion is characterized by the thermodynamic anomalies associated with the quark-hadron phase transition. Due to these anomalies the composite rarefaction wave including the rarefaction shock as a component arises. The behaviour of the rarefaction shock being the hadronization wave is of special interest. It is shown that the reflection of the rarefaction wave in the quark-gluon phase from the symmetry axis (plane) results in the formation of inner hadronization wave, which propagates from the center of the fireball to its periphery. Interference of the hadronization wave with the entropy nonuniformities leads to the spatial fragmentation of the two-phase region.

Instability and oscillatory modes of multiphase flow in a porous medium with reactive skeleton

Konyukhov A V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

konyukhov_av@mail.ru

Injection of oxidizer into the porous medium with reactive skeleton is a part of advanced heavy oil production technologies, such as in-situ combustion. The front of the oxidation reaction in the porous medium is known to exhibit instabilities, which have multidimensional (fingering) or one-dimensional nature. In the latter case, the reaction rates, phase saturations, pressure etc. are subjected to quasi periodical oscillations. This kind of instability has been studied using the laboratory experiment [1]. The characteristic feature of the instability under consideration is "cold' mechanism of positive feedback, which makes it possible for the low-temperature reactions. In the present work the mathematical model of the reactive multiphase flow is formulated which takes into account the multiphase transport, one-step chemical reaction, change of porosity and permeability due to the reaction. The development of the instability and its dependence on the flow parameters are investigated.

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From difference to similarity in shock-induced ejecting from metals simulated by molecular-dynamics and smoothed-particle-hydrodynamics methods

Dyachkov S A[1,2,@], Egorova M S[1], Parshikov A N[1] and Zhakhovsky V V[1]

[1] All-Russia Research Institute of Automatics named after Dukhov, Luganskaya 9, Moscow 115304, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] serj.dyachkov@gmail.com

The microscopic jets can be generated from the material with surface corrugations under shock loading [1]. The space–time evolution of such jets is difficult to obtain in experiment. However, the process of jet formation can be observed in simulations by molecular dynamics (MD) [2, 3] and hydrodynamics methods [4]. Because jetting is accompanied by a dramatic deformation and fragmentation of material, it can be effectively simulated by smoothed particle hydrodynamics (SPH), which is a mesh-free Lagrangian method. Here we study similarity between jets obtained in consistent MD and SPH simulations. We demonstrate good agreement between both methods for strong enough shocks: the scaling provides the similar jet velocity profiles and mass distributions. However for weaker shocks and small surface corrugations the scaling does not work well. Both material strength and surface tension reduce ejecta velocity at atomic scales, but their effect decreases with increase of MD sample size leading to better agreement.

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Molecular dynamic investigations of the shock pulses interaction with free target surface with nanostructure

Ebel A A[1,2,@] **and Mayer A E**[1]

[1] Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia
[2] South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia

[@] ebel_aa@rambler.ru

High-speed impact or intensive irradiation generates in material a compression pulse, which is a shock wave followed by a release wave. Reflection of the compression pulse from a free surface of material leads to formation of a tension wave propagating in the inverse direction. Action of tensile stresses can results in the spall fracture. If the free surface is not a flat one and has some protrusions or troughs comparable in size with the compression pulse thickness, the uniaxial strain state typical for flat shock waves is changed on a more complex strain state at interaction with these surface relief elements. As a result, a part of the compression pulse energy dissipates due to an intensive plastic deformation in this surface layer. It leads to a decrease of the tensile wave amplitude and, consequently, an increase of the spallation threshold in terms of the incident shock wave intensity. In this report, by an example of copper and by means of molecular dynamics simulations, we investigate the influence of the surface nanorelief on the spallation threshold under the action of short compression pulses.

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Continuum model of tensile fracture of metals and its application to the shock wave problems

Mayer A E

Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia

mayer@csu.ru

A continuum model of tensile fracture of solid metals is formulated and verified within a wide range of strain rates and temperatures using results of MD simulations and known experimental data. The model considers as competitive processes the growth of voids of two different shapes—the cylindrical cracks and spherical voids. Both thermo-fluctuational nucleations of new voids and growth of the pre-existing ones are considered. The model is applied to description of the back-side spallation of metal targets exposed to the shock wave loading initiated by high-speed impact and high-current electron irradiation; calculations are performed in both 1D and 2D cases. Results of comparison with known experimental back surface velocity histories are presented. Influence of initial structural heterogeneities of material, such as non-uniform dislocation density distribution, presence of inclusions and pre-existing voids, is analyzed. The work was supported by the grant from the Russian Science Foundation (Project No. 14-11-00538).

Molecular dynamics and continuum modeling of nanopore growth in copper at high-rate tension

Latypov F T[@], Krasnikov V S and Mayer A E

Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia

[@] latypovfanil@gmail.com

Destruction of metals occurs by two mechanisms: (i) the ductile fracture realized by means of the nucleation, growth and coalescence of voids; (ii) the brittle fracture realized by means of the formation and growth of cracks as a dominant process [1]. Attention to the plastic deformation near the voids and cracks is due to the assumption of the dislocation stimulated growth of them [2]. A two-level model of the dislocation-stimulated growth of nanopores in aluminum is proposed in [3] in order to predict the critical pressure of fracture. The nanopores growth is connected with the plastic deformation in the region close to the pore leading to the atoms rearrangement on the pore surface. It was decided to continue the work and apply the proposed model [3] to the copper. In our report, the results of molecular-dynamics simulations in comparison with the continuum model are presented.

The work was supported by the grant from the Russian Science Foundation (project No. 14-11-00538).

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Molecular dynamics investigation of nucleation rate of nanopores in aluminum at negative pressure

Voronin D S[@], Krasnikov V S and Mayer A E

Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia

[@] v-demonizerus@mail.ru

In this report we present the results of molecular-dynamics (MD) verification of the formula proposed in [1] for calculating the nucleation rate of nanopores in metals at negative pressure. Using molecular dynamics the formation of pores in solid aluminum in an extended state was studied. The sample lifetime was determined at a temperature of 300 K and various pressures with taking into account the statistical straggling. The calculations were performed using the program LAMMPS [2] and the interatomic potential AL99 [3]. Sample contained 256000 aluminum atoms formed in a cubic body, the temperature of 300 K was maintained constant by a thermostat, a negative pressure is maintained by the barostat. Step of time integration was 0.001 ps, the system was traced for 400 ps. Several MD trajectories were simulated different trajectories were set by varying the initial velocity distribution of atoms. The dependence of nucleation rate on pressure was plotted according to the data of MD simulations. The work was supported by the grant from the Russian Science Foundation (project No. 14-11-00538).

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Numerical simulation of dynamic failure and multi spall fracture in metals

Bayandin Yu V[@], Saveleva N V and Naimark O B

Institute of Continuous Media Mechanics of the Ural Branch of the Russian Academy of Sciences, Academician Korolev Street 1, Perm 614013, Russia

[@] buv@icmm.ru

Dynamic behavior of metals under intensive loading is characterized by intensive nucleation and growth of defects (microshears and microcracks) both under shock-wave compression and unloading conditions that may reduce to spallation and in some cases to multiple spallation. Spall fracture in material produced by the action of tensile stress in bulk of sample when two decompression waves collide. For higher amplitudes of shockwave the initiation of secondary spallation appears when intensity of residual wave is enough. The purpose of present investigation is consists on formulation of physical-mathematical model of dynamic behavior of metals under shock compression loadings. Plate impact test is considered. Wide range constitutive model based on the statistical theory for solids with defect (microshears and microcracks) was developed.

Fractoluminescence of granite under plate impact

Uvarov S V[@], Panteleev I A and Naimark O B

Institute of Continuous Media Mechanics of the Ural Branch of the Russian Academy of Sciences, Academician Korolev Street 1, Perm 614013, Russia

[@] usv@icmm.ru

Fractoluminescence of granite under plate impact was investigated. Granite samples 50 mm long with crossection 100×50 mm^2 were loaded by 5 mm thick mild steel flyer at velocities upto 300 m/s. Fractoluminescence was detected by Hamamatsu PMT placed at 300 mm from a lateral side of the specimen so we can register luminescence events from all lateral surface faced to the PMT thus we have no spatial resolution. Output from the photomultiplier tube was recorded by Tektronix DP07254 digital oscilloscope. It was found that luminescence lasts for tens of milliseconds while compressive wave propagation time is 10 μs which is three orders shorter. First pulse with sharp front is related to the impact event. Next pulse starts at 80 μs after and lasts for 60 μs. It has a smooth shape and can be related to the spall failure. Then, after 1ms we have observed lots of weak short pulses same as we have observed in our experiments on the split hopkinson bar [1]. But after 1ms the granite target or its fragments can hit other metallic parts of the experimental setup so we need further investidation of the nature of these pulses.

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Research of fracture of materials and designs at shock-wave loadings by means of the program complex EFES

Radchenko P A[1], Radchenko A V[1,@], Batuev S P[1] and Tukaev A M[2]

[1] Tomsk State University of Architecture and Building, Solyanaya Square 2 Bldg 2, Tomsk 634003, Russia
[2] Joint Stock Company Research and Production Corporation "Konstruktorskoye Byuro Mashinostroyeniya", Okskiy Street 42, Kolomna, Moscow Region 140402, Russia

[@] andrey-radchenko@live.ru

The results of coordinated experimental and numerical studies of destruction of materials and structures under impact. Numerical simulation is carried out by the author finite element software package EFES, allowing to simulate a three-dimensional setting behavior of complex structures under dynamic loads. Investigated the destruction of metallic and nonmetallic materials and structures are in the speed range of interaction 50–3000 m/s. A comparison with experimental data.
This work was partially supported by RFBR grants 16-31-00125, 16-38-00256.

Numerical simulation of concrete structures with anisotropic non-metal reinforcement at impulse loadings

Batuev S P[@], Radchenko P A, Radchenko A V, Plevkov V S and Kudyakov K L

Tomsk State University of Architecture and Building, Solyanaya Square 2 Bldg 2, Tomsk 634003, Russia

[@] spbatuev@gmail.com

Results of the study on the operation of the reinforced concrete and fiber-reinforced concrete with metal and non-metallic fiber reinforcement under short-term dynamic loading are presented in the paper. Program of experimental and numerical studies was developed. Mathematical and numerical simulation is carried out to the full three-dimensional setting, taking into account the real properties of materials and constructions: anisotropy, plasticity, viscosity, kinetic nature of fracture, the various values of the elastic and strength properties under compression and tension, the influence of the loading rate on the physical and mechanical properties of materials. As a result of experimental studies schemes of deformation, cracking and fracture, as well as values of fracture loads of experimental samples were obtained. Present results are compared with data of the numerical calculations performed using the computational program based on finite elements method. Results of experimental and numerical calculations showed good convergence.

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Two-dimensional modeling of high-speed impact of polymethylmethacrylate plates

Popova T V[1,@], Mayer A E[1] and Khishchenko K V[2]

[1] Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia

[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] tatyana_maskaeva@mail.ru

We perform two-dimensional simulation of the polymethylmethacrylate plates impact (PMMA) using Maxwell model of viscoelastic medium. Previously, we investigated the influence of the viscoelastic properties on the shock wave dynamics in PMMA in one-dimensional calculation [1]. It was shown that, in a limit of weak shock waves, the accounting of the viscoelastic properties allows one to achieve a better coincidence of the calculated and experimental data on the shock wave velocity magnitude in comparison with the case of hydrodynamic calculations. In the present work, we have generalized the polymeric material deformation model to the case of two-dimensional stress state. A relation is written for the relaxation of shear stresses in the plane, in which the maximum tangential stress acts. Parameters of the Maxwell model are chosen by comparison with the experimental data [2–4]. A caloric equation of state is used to calculate the pressure from density and internal energy [5, 6].

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The fabrication of boron carbide compacts by explosive consolidation

Buzyurkin A E[1,@], Kraus E I[1] and Lukyanov Ya L[2]

[1] Institute of Theoretical and Applied Mechanics of the Siberian Branch of the Russian Academy of Sciences, Institutskaya 4/1, Novosibirsk 630090, Russia
[2] Lavrentyev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 15, Novosibirsk 630090, Russia

[@] buzjura@itam.nsc.ru

In this paper experiments on explosive consolidation of powdered boron carbide and numerical modeling of the stress state behind the shock front were carried out. The aim of this study was to obtain a durable compacts with low porosity. Explosive consolidation was used in this problem because the boron carbide is an extremely hard and refractory material. Therefore, the use of traditional methods require special equipment and considerable expenses.

Sound velocity measurements in shock compressed Ni+Al mixture samples of micro- and nanodispersed components

Yakushev V V[1,@], Utkin A V[1], Dolgoborodov A Yu[2], Ananev S Yu[2] and Zhukov A N[1]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] yakushev@ficp.ac.ru

Ni+Al-system belongs to so-called reactive materials which are able to react with significant thermal flux in condenced state. The potentiality of these systems to react on a microsecond scale under shock-wave loading is of great interest. Nevertheless recent experiments on shock compression [1] showed that main power flux in a volume starts much later than the moment of compression (tens and hundreds of microseconds). At the same time it remains unclear if the reaction proceeds to any visible extent during existence of high pressure ($\sim$ 1 mks). In the present work we measured sound velocity depending on pressure for Ni+Al mixture samples of micro- and nanosized components. Since sound velocity is very sensitive to the state of a matter it can be useful to identify the processes occuring in the material, for example chemical reactions.

The time of sound wave propagation through the sample was depended from shock wave profiles registered using VISAR. It was shown that for samples prepared from nanomixtures sound velocity is 20–30% higher than for those prepared using microdispersed mixtures. The effect can be caused not only by the volume reaction but most probably by the higher amount of Al_2O_3 in nanomixture. The explanation of real nature of the effect requires deeper investigation.

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Detonability of mechanoactivated ammonium-perchlorate-based mixtures with nano-Al

Shevchenko A A[1,2,@], Dolgoborodov A Yu[1,3,2], Brazhikov M A[2] and Kirilenko V G[2]

[1] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[2] Semenov Institute of Chemical Physics of the Russian Academy of Sciences, Kosygina 4, Moscow 119991, Russia
[3] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] arsshevchenko@inbox.ru

In the present work, detonation ability of Al/ammonium perchlorate (AP) (20/80) high-dense charges has been studied. The pressed charges were produced from preliminary mechanochemically activated AP-based mixtures—AP 50–100 μm in size and Al powders: Alex 150–200 nm in size, and pyrotechnic powder PP-2 (50–200 μm $\times$ 2–5 μm). It was experimentally showed that detonability of activated Al/AP mixtures could be shifted into the area of higher densities at small charge diameters. For 25-mm charges $D(\rho)$-dependence demonstrated the maximum D-value for Alex-containing mixture at 0.91 TMD, while for PP-2 the maximum was observed at 0.75 of TMD. For activated Alex-based composition (0.75 of TMD), there was obtained nonlinear $D(1/d)$-dependence. D increased with d growth from d = 10–17 mm, the velocity remained constant at d = 17–40 mm with consequent growth at $d \geq 40$ mm. At d = 50 mm, D was measured to be the same as it was obtained for PP-2-containing compositions. Such detonation mode is named pseudo-ideal detonation. The maximum on detonation velocity $D = 6.4$ km/s was obtained at 0.9 of TMD and $d = 40$ mm. Experimental data on D measured for mechanoactivated mixture with Alex, exceed those for non-activated mixtures with Alex and activated mixtures with PP-2. This work was supported by RFBR (grant No. 16-29-01030) and the Program of fundamental researches of the Presidium RAS "Thermal physics of high energy density".

The comparison of shock wave absorption in porous reactive materials

Ananev S Yu[1,2,@], Dolgoborodov A Yu[1], Shiray A A[2] and Yankovsky B D[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] serg.ananev@gmail.com

Experiments on impact loading of the pressed samples from different thermite compositions are described. Thermite structures are the reactive materials, which are capable to the components exothermic interaction under shock wave loading. We used the mechanoactivated metal and oxide powders as components of thermite compositions. Shock loading of the thermic tablets was performed by the detonation of the explosive charge in a steel cylindrical shell through an inert spacer. Finally, the steel barrier deformed in the point of shell fixing. The volume of a barrier's material residual deformation is connected with amount of primary shock wave energy, which reached a barrier. For identical loading conditions of thermite tablets, made from various components, the amount of energy reached a barrier depends on extent of energy dissipation in these tablets. Energy dissipation in thermite tablets occurs due to deformation and mutual movement of initial components particles. Deformation of particles and surface friction at their mutual movement is accompanied by the conversion of shock wave energy into heat. To quantify the shock wave energy losses conducted a series of experiments in which thermite tablet was replaced by a dense spacer made of inert material of known specifications. Thus, comparing a steel barriers deformation it is possible to estimate in relative units the energy losses for different tablets under loading. In relative units this energy losses were 55–98% for different thermite compositions. The experiments described precede study of shock initiation of chemical transformations in thermite compositions.

Detection of micro- and nanoparticles in dynamic processes

Ten K A[1,@], Pruuel E R[1], Kashkarov A O[1], Rubtsov I A[3], Shechtman L I[2], Zhulanov V V[2], Tolochko B P[2], Rykovanov G N[4], Muzyrya A K[4], Smirnov E B[4], Stolbikov V Yu[4] and Prosvirnin K M[4]

[1] Lavrentyev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 15, Novosibirsk 630090, Russia
[2] Budker Institute of Nuclear Physics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 11, Novosibirsk 630090, Russia
[3] Novosibirsk State University, Pirogova Street 2, Novosibirsk 630090, Russia
[4] Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia

[@] ten@hydro.nsc.ru

In a shock impact on a metal plate, particles of various sizes are emitted from the free surface (shock-wave "dusting"). The particle sizes range from a few microns to hundreds of microns [1]. The particle flow was assumed to include finer particles too, but the existing techniques cannot resolve them yet.
BINP have commissioned SYRAFEEMA (Synchrotron Radiation Facility for Exploring Energetic Materials), which enables measurement of small-angle x-ray scattering (SAXS) of synchrotron radiation (SR) from the collider VEPP-4M (energy of 4 GeV). The SR SAXS technique and precision measurement of passed SR were applied to studies of flows of nano- and micro-particles from free surface of various materials (copper, tin, and tantalum). Flows of nanoparticles were detected for the first time in impact of pressed HMX on foil of tin and tantalum. The density distributions along the microjets formed from micron-sized slots were obtained.

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Dynamics of sizes of nanoparticles at trinitrotoluene detonation on the VEPP-4M synchrotron radiation

Rubtsov I A[1,2,@], Ten K A[1], Pruuel E R[1,2] and Kashkarov A O[1,2]

[1] Lavrentyev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 15, Novosibirsk 630090, Russia
[2] Novosibirsk State University, Pirogova Street 2, Novosibirsk 630090, Russia

[@] rubtsov314@mail.ru

Registration of small angle x-ray scattering (SAXS) during detonation of high explosives (HE) allows to measure fluctuation of density in a zone of chemical reaction. In the case of oxygen-deficient HEs it is connected with synthesis of condensed carbon phases—ultradisperse diamonds (UDD) or graphite.
In this work we carried out SAXS measurement during trinitrotoluene (TNT) detonation. SAXS simulation with real spectrum (the viggler radiation, TNT absorption, absorption of the DIMEX-3 detector) was performed. Comparison of calculated and measured SAXS distribution allows to obtain dynamics of average sizes of nanodiamonds behind the detonation front using pink SR beam.
Experiments with using SR were made on SYRAFEEMA (Synchrotron Radiation Facility for Exploring Energetic Materials) station at the accelerating complex VEPP-4M (Budker Institute of Nuclear Physics). This new station allows to increase the mass of the studied charges by 10 times to 200 grams in comparison with similar station "Extreme states of matter" at the accelerating complex VEPP-3.

Transmission electron microscopy and x-ray diffraction studies of high explosives detonation soot

Kashkarov A O[1,2,@], Pruuel E R[1,2], Ten K A[1], Rubtsov I A[1,2], Gerasimov E Yu[3,2] and Zubkov P I[1]

[1] Lavrentyev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 15, Novosibirsk 630090, Russia
[2] Novosibirsk State University, Pirogova Street 2, Novosibirsk 630090, Russia
[3] Boreskov Institute of Catalysis of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 5, Novosibirsk 630090, Russia

[@] kashkarov@hydro.nsc.ru

Electron microscopy and diffraction studies were performed on the saved condensed detonation products of a number of high explosives (HEs): TNT, composition TNT/RDX (50/50), BTF (benzotrifuroxan) and TATB.
The samples were 20 mm in diameter and 30 mm in length, and weight is about 20 g. The detonation was initiated by PETN or HMX, as those HEs produce inessential amount of detonation soot. The experimental samples was placed in 1 kg ice shell.
The uniform experimental conditions allows to to conduct a qualitative and quantitative comparison of obtained under similar conditions detonation soot of various HEs. The results demonstrates differences in graphite-like and diamond inclusions morphology and quantitative content of nanodiamonds for selected HEs.

Instability of detonation waves in FEFO/methanol mixtures

Utkin A V[1,2,@], Mochalova V M[1,2], Torunov S I[1] and Koldunov S A[1]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] Tomsk State University, Lenina Avenue 36, Tomsk 634050, Russia

[@] utkin@icp.ac.ru

In liquid HE, detonation waves propagate both in steady and unsteady pulsating regimes. At that it should distinguish the loss of stability of one-dimensional flow, which occurs at the absence of influence of the boundaries, and instability at the edge of the charge. The purpose of this work is to prove that, in practice, the relationship between these two types of instability is not strictly determined. We studied bis-(2-fluoro-2.2-dinitro-ethyl)-formal (FEFO, $C_5H_6N_4O_{10}F_2$) and the mixtures of FEFO with methanol. The structure of the detonation wave was recorded by a VISAR interferometer and by high-speed streak camera. It was found strong velocity oscillations in both the chemical reaction zone and the unloading wave for FEFO. This implies that the detonation front is unstable. According to the generally accepted concept, reaction failure waves should be observed also. However it was found that the boundary at the edge of the charge is smooth, without evidence of the existence of reaction failure waves. Dilution of FEFO by methanol results in qualitative changes in the nature of flow in detonation waves of the mixture. When the methanol concentration changes in the interval 10–20%, the stabilization of detonation front is observed and reaction failure waves are occurred at the edge of the charge. Further increase of the concentration of the inert diluent results in the instability of the detonation front at existing of the reaction failure waves. Obtained results show, therefore, that the reaction failure waves and stability of one-dimensional detonation front appear, in general, independently. This work was supported by Russian Foundation for Basic Research (project 15-03-07830).

Experimental investigation of cylindrical detonation wave

Dudin S V, Sosikov V A[@] and Torunov S I

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] vaso@icp.ac.ru

Cylindrical detonation wave is widely used as for fundamental investigation in high-pressure physics [1, 2] and for solving practical problems. Cylindrical or conical detonation wave is used in electrodynamical devices of various types [3], in pulse generators of high pressure [4], cumulative devices [5], in special charges for imploding works. Interesting features of gasdynamic flows of detonation products were first discovered during formation of cylindrical detonation wave using multipoint initiation method. This features, which consist of the formation of complex system of shock waves with cell structure after the detonation wave, are force us to take a closer look to dynamic of formation of detonation waves and flow of detonation products. This cell structure persist during the entire time of the convergence of detonation waves, i.e. longer than 10 μs. Triple wave Mach configuration must be forms in points of conjugation of neighboring detonation waves that must be lead to alignment of front. Use of modern methods of pulse processes diagnostics (high-speed photography with nanosecond time resolution) will let us to carry out research at the highest level [1].

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Mathematical modeling of converging detonation waves in a multi-point initiation

Shutov A V[@], Sultanov V G and Dudin S V

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] shutov@ficp.ac.ru

Cylindrical detonation wave and the motion of cylindrical piston to the center is quite well studied [1–5]. In experimental studies in IPCP RAS [6], which uses cylindrical or conical detonation wave is formed by the method of multipoint initiation, were found some features of gas-dynamic flow of the detonation products. The article suggests a mathematical model of cylindrical detonation, consistent with experimental results. Mathematical modeling of cylindrical detonation waves taking into account the kinetics of decomposition significantly reduces the number of costly explosive experiments. The combination of experimental studies together with the results of numerical simulation let us obtain an adequate picture of the development of various types of detonation waves (planar, cylindrical, conical, and spherical) under multipoint initiation.

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Detonation model for non-ideal condensed explosives

Smirnov E B[@], Kostitsyn O V and Koval A V

Federal State Unitary Enterprise "Russian Federal Nuclear Center—Academician Zababakhin All-Russian Research Institute of Technical Physics", Vasilieva 13, Snezhinsk, Chelyabinsk Region 456770, Russia

[@] ewgeny_smirnov@mail.ru

The Zeldovich–Neumann–Doering theory of ideal detonation can adequately describe the detonation of charges with near-critical diameter. For minor diameters, detonation velocity can differ significantly from an ideal value expected based on equilibrium chemical thermodynamics. This difference is quite evident when using non-ideal explosives; in certain cases, this value can be up to one third of ideal detonation velocity. Numerical simulation of these systems is a very labor-consuming process because one needs to compute the states inside the chemical reaction zone, as well as to obtain data on the equation of state of HE-explosion products mixture and on the rate of chemical reaction; however, these characteristics are poorly studied today. For practical purposes, one can use the detonation shock dynamics model based on interrelation between local velocity of the front and its local curvature. This interrelation depends on both the equation of state of explosion products, and the reaction rate; but the explicit definition of these characteristics is not needed.
In this paper, experimental results are analyzed. They demonstrate interrelation between the local curvature of detonation front and the detonation velocity. Equation of detonation front shape is found. This equation allows us to predict detonation velocity and shape of detonation wave front in arbitrary geometry by integrating ordinary differential equation for the front shape with a boundary condition at the charge edge. These results confirm that the model of detonation shock dynamics can be used to describe detonation processes in non-ideal explosives.

Detonation initiation in AB model of explosive: Comparative atomistic and hydrodynamics simulations

Murzov S A[2,1,@], Sergeev O V[1], Dyachkov S A[2,1], Egorova M S[1], Parshikov A N[1] and Zhakhovsky V V[1]

[1] All-Russia Research Institute of Automatics named after Dukhov, Sushchevskaya 22, Moscow 127055, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] semen.murzov@phystech.edu

As atomistic simulation indicates, the thermal decomposition of condensed phase explosive PETN and AB model explosive is initiated by chemical reactions within a picosecond timescale after several atomic oscillations. We developed the kinetic model [1, 2] of chemical reactions observed in a molecular dynamics (MD) simulation of self-sustained detonation wave [2] with the aim to use the model in hydrodynamic simulation of detonation initiation. Kinetic coefficients are obtained by minimization of difference between profiles of species calculated from the kinetic model and observed in MD simulations of isochoric thermal decomposition with a help of downhill simplex method combined with random walk in multidimensional space of fitting kinetic coefficients. Here we present the consistent MD and smoothed particle hydrodynamics (SPH) [3] simulations of detonation where reaction rates and equation of state used in SPH has been obtained from MD simulation of AB model explosive. Difference and similarity between MD and SPH results are demonstrated. Extension of developed kinetic model on SPH modeling of PETN explosive is discussed.

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The method of calculating the thermodynamic properties and the composition of the explosion products if there is no full chemical equilibrium

Shargatov V A[@] and Gubin S A

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

[@] shargatov@mail.ru

The chemical reactions that occur in the chemically non-equilibrium explosion products change their composition and, consequently, thermodynamic parameters. At a large number of individual species in the explosion products and a large number of chemical reactions involved, calculation of the mixture composition requires a long computation time. An approximate method for calculating composition of the non-equilibrium mixture of explosion products is developed. The method is based on a physically reasonable assumption that equilibrium in the almost all bimolecular reactions is established much faster than the full chemical equilibrium, being applicable when this assumption holds. The method uses the assumption of the existence of maximum of entropy for a given density, internal energy, molecular weight of the detonation products mixture and some linear combination of concentrations. Without significant loss of accuracy to the solution of stiff differential equations detailed kinetic mechanism can be replaced by one or two differential equation and a system of algebraic equations. This method is always consistent with the detailed mechanism and can be used separately or in conjunction with the decision of a stiff system for chemically non-equilibrium mixtures replacing it when almost all bimolecular reactions are near to equilibrium. It was shown that the proposed model can be used to calculate the characteristics of the chemically non-equilibrium explosion products of acetylene-oxygen mixture.

Universal concept of the unique magnetodipole holographic spectrum of the energetic materials reactionary zones

Lukin A N

Western-Caucasus Research Center, Tupik Zvezdniy 9, Tuapse, Krasnodar Territory 352808, Russia

lukin@wcrc.ru

In accordance with our novel microscale combustion concept, motivated excitation source of the 3D micro/nanoscale physical structures in the reactionary zones are the micro/nanoscale structures of the electromagnetic fields. According to our challenging hypothesis each energetic material has a unique interactive magnetodipole (electromagnetic) holographic spectrum of the reactionary zone which is the synergetic oscillatory system. Such synergetic system also can be characterized by the frequency code. Our hypothesis is supported by the recent data, obtained in the various model combustion systems. Magnetodipole 3D micro/nanoscale structures can be considered as information medium which characterizes the reactionary zone of the energetic material. Instead of using laser-assisted combustion (laser heating of the solid propellant surface) where thrust is variable by adjusting laser power, we suggest excitation of the resonance spectrums of the reactionary zones by means of polarized (resonance) laser radiation. Additional effects can be obtained by laser-induced self-organizing of the 3D micro/nanoscale structures in the reactionary zones. Also the techniques of scanning (reading) by laser radiation of the unique holographic spectrums of the energetic materials reactionary zones are considered. Laser-induced excitation of these spectrums along with reprogramming of the magnetodipole spectrum of the reactionary zones gives the possibility for control by the scale and 3D localization of the induction and energy-releasing areas and, accordingly, allows control interscale interaction in the aerospace propulsion systems.

Using explosive technologies to create a compact current-limiting device rated for operation on 110 kV class systems

Shurupov A V, Shurupov M A, Kozlov A A[@] and Kotov A V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] alexk5577@yandex.ru

This paper considers the possibility of creating on new physical principles a high-speed current-limiting device (CLD) for the networks with voltage of 110 kV, namely, on the basis of the explosive switching elements. The device is designed to limit the steady short-circuit current to acceptable values for the time does not exceed 3 ms at electric power facilities. The paper presents an analysis of the electrical circuit of CLD. The main features of the scheme are: a new high-speed switching element with high regenerating voltage; fusible switching element that enables to limit the overvoltage after sudden breakage of network of the explosive switch; non-inductive resistor with a high heat capacity and a special reactor with operating time less than 1 second. We analyzed the work of the CLD with help of special software PSPICE, which is based on the equivalent circuit of single-phase short circuit to ground in 110 kV network. Analysis of the equivalent circuit operation CLD shows its efficiency and determines the CLD as a perspective direction of the current-limiting devices of new generation. CLD class 110 kV meets all the requirements, provided for a new class of devices and could be one of the key components of security of electricity networks in the future.

Characteristic features of the chemiluminescent emission of CH^*, C_2^*, OH^* and CO_2^* caused by ethane ignition behind reflected shock waves

Vlasov P A[1,2,@], Tereza A M[1], Smirnov V N[1], Shumova V V[3,1], Atkin E V[2] and Demidenko T S[2]

[1] Semenov Institute of Chemical Physics of the Russian Academy of Sciences, Kosygina 4, Moscow 119991, Russia
[2] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[3] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] iz@chph.ras.ru

The experiments have been carried out on the simultaneous measurements of the emission of CH^*, C_2^*, OH^*, and CO_2^* during self-ignition of various mixtures of ethane with oxygen and argon behind reflected shock waves within the temperature range of 1280–1790 K for the total mixture density of $(1 \pm 0.2) \times 10^{-5}$ mol/cm^3. It was shown that the time of emission maximum practically coincides for all radiating species being recorded. The characteristic features of the time dependences of the intensity of OH^* emission were revealed depending on the temperature and mixture stoichiometry. Practically symbate behavior of the profiles of CH^*, C_2^*, and CO_2^* emission was demonstrated within the ranges of temperature, pressure and ϕ under study. The results of numerical modeling are in good agreement with our experimental results.

Kinetics of hydrogen oxidation at the early stages of induction period behind reflected shock waves

Tereza A M[1,@], Agafonov G L[1], Atkin E V[2], Medvedev S P[1], Smirnov V N[1] and Vlasov P A[1,2]

[1] Semenov Institute of Chemical Physics of the Russian Academy of Sciences, Kosygina 4, Moscow 119991, Russia
[2] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

[@] atereza@bk.ru

In the current work the experiments were performed on record of the chemiluminescent emission of OH^* radicals ($\lambda = 308$ nm) within the temperature range of $800 < T < 1000$ K at the early stage of the induction period at a pressure of 0.1 MPa. These experimental conditions make it possible to measure OH^* emission for the time intervals less than 1 ms, when the influence of physical-chemical factors capable to influence the homogeneous development of the self-ignition process is minimal. Thus, it was possible to avoid the influence of early appearance of the self-ignition places, the pressure rise, caused by deceleration of the incident shock wave or the arrival of disturbances from the contact surface. The results of experiments showed that at the early stage of the induction period the process of H_2 oxidation proceeds by chain-branching reactions with the branching factor ϕ. To reveal the specific features of the kinetic mechanism of high-temperature hydrogen oxidation, we developed the corresponding kinetic mechanism, validated both on our own experimental results and on the results of various authors on records of O, H, OH radicals and water molecules within a wide temperature (950–2500 K) and pressure (0.05–0.85 MPa) range for different initial concentrations and in various bath gases. The numerical modeling of OH^* emission at the early stages of H_2 oxidation showed that to describe the temperature dependence of ϕ-factor it is necessary to take into account the quantum corrections in the initiation reactions of a H_2/O_2 system.

The study of kinetics of Br atom formation at the pypolysis of $C_2F_4Br_2$ behind shock waves

Emelianov A V[1,@], Eremin A V[1] and Yatsenko P I[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] aemelia@ihed.ras.ru

Various halogenated hydrocarbons are widely used for the fire fighting. 1,2-dibromotetrafluoroethane ($C_2F_4Br_2$) is one of the most widely used in Russia fire extinguishing compounds. Azatyan *et al* [1] reported that combustion suppression takes place due to chemical inhibition of chain combustion reactions. It is assumed that Br is the primary product of the $C_2F_4Br_2$ dissociation and it is responsible for the suppression of chain reactions of combustion. However, the kinetics of decomposition of $C_2F_4Br_2$ is studied very superficially [2]. Therefore, the main goal of this work is to study the kinetics of formation Br atom and to trace the possibility of CF_2 radical in the pyrolysis $C_2F_4Br_2$ of shock waves.

The study of the kinetics of formation and consumption of Br atoms behind shock waves was carried out by the method of atomic resonance absorption spectroscopy (ARAS) using vacuum-uv lines of Br-atom in the range of 148–165 nm. The initial concentrations of Br_2 or $C_2F_4Br_2$ in argon were varied from 0.002 to 1.0%. The time dependence of Br atom concentration in the pyrolysis of Br_2 and $C_2F_4Br_2$ at the temperatures from 2500 to 4000 K and the pressures from 2 to 17 bar behind reflected shock waves were measured. From these data the temperature dependence of the dissociation rate constant of $C_2F_4Br_2$ at different pressures was determined.

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Temperature measurements of combustible mixtures behind shock waves

Matveeva N A[1,2,@] **and Mikheyeva E Yu**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] nataliematveeva1@gmail.com

The experiments were conducted in methane- and acetylene-oxygen mixtures with chemical additives of CCL_4 and CF_3H. The emission-absorption diagnostics, used for temperature measurements, was tested in non-reactive mixtures of carbon dioxide and oxygen diluted in argon. Experiments were carried out behind the reflected shock waves in the temperature range of T5=1700-3080 K and pressure range of P5=6-8 bar for non-reactive mixtures and in range oftemperature T5=1270-1930 K and pressure P5=4.7-5.5 bar for combustible gases. In these experiments the dependence of the ignition delay times and the temperature behavior in the combustion zone on the mixture concentration and on the presence of additives were measured. The experimental data of temperature dependence of ignition delay times were compared with the results of calculation by theChemkin-Pro package using kinetic mechanisms [1]. It was found that measured temperature in the combustion zone did not depend on the initial parameters behind the reflected shock wave. The addition of CF_3H to methane-oxygen mixtures had no effect on the value of the temperature in the combustion zone, while the addition of CCL_4 decreased the temperature down to 200K because of the heat consumption inthe decomposition of CCL_4. These experimental data can be used for testing and development of kinetic schemes of ignition and combustion of methane and acetylene in the presence of perspective inhibitors. This work has been supported by the Russian Science Foundation (project No. 14-19-00025).

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Experimental study of reaction $CO+O_2=CO_2+O$ behind shock waves

Drakon A V[1], Emelianov A V[1], Eremin A V[1] and Yatsenko P I[1,2,@]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] mr.pavl1kk@gmail.com

The reaction $CO+O_2=CO_2+O$ (1) plays an essential role in the process of ignition of synthesis gas and other fuels containing carbon monoxide. The peculiarity of this reaction is very high activation energy with practically zero heat effect that gives rise to serious controversies in the available experimental data, and in their theoretical interpretation. Therefore despite large number of works [1] carried out hitherto, comprehensive data on the kinetics of this reaction was not available. Sometimes the rate constants are different by orders of magnitude. In this work the experimental study of kinetics of $CO+O_2$ reaction using ARAS in vacuum UV range at a wavelength λ=130.5 nm was performed behind reflected shock waves. More than 30 successful experiments in the temperature range $1300 \leq T_5 \leq 2000$ K and pressure range $2.5 \leq P_5 \leq 17$ bar in the mixture $0.1\%O_2+0.1\%CO+Ar$ were carried out. From the experimental data the temperature dependencies of the reaction rate constant were determined at different pressures. The activation energy of this reaction was found, which equals 240 kJ/mole. For the first time it was found that the increase in pressure of the diluent gas leads to suppression of reaction (1), which may be regarded to the processes of quenching of the activated complex ($CO{:}O_2$), formed in the collisions $CO+O_2$, and the acceleration of the reverse reaction $O+CO_2$ due to the quantum corrections to the rate constants of chemical reactions [2].

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Carbon nanoparticles temperature measurements by four-colour laser-induced incandescence

Mikheyeva E Yu[1,2] **and Selyakov I N**[1,2,@]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] ivan_sel@yahoo.com

This study is devoted to the temperature measurements of carbon nanoparticles formed in shock tube and heated by laser pulse. The nanoparticles were synthesized after heating a mixture of 0.5% of benzene and argon by a shock wave. The conditions behind the reflected shock wave were P_5 = 4–5 bar and T_5 = 1600–2400 K. The heating of nanoparticles was initiated by Nd:YAG laser pulse at 1064 nm, fluence of 0.3–0.4 J/cm^2 and duration of pulse of 10 ns. Nanoparticles temperature was measured by two-colour pyrometry using laser-induced incandescence (LII) signals. LII is a method, based on analyzing the thermal radiation of particles heated by laser pulse. The nanoparticles cooled due to colliding with the molecules of surrounding gas, sublimation and heat radiation. The radiation, emitted by nanoparticles was converged through the front diagnostic window by a lens, and passing through a semitransparent mirror and optical filters (772 and 550 nm), was collected by two photomultipliers. For the first time two more photomultipliers with optical filters of 488 and 610 nm were attached to diagnostic sidewall windows by both sides of the shock tube. The measurements from sidewall windows turned out to be more sensitive that helped to improve temperature measurements of carbon nanoparticles. Moreover, the simultaneous measurements of four LII signals can help to find out new information of wavelength dependence of optical properties of carbon nanoparticles. This work has been supported by the Russian Foundation for Basic Research (grant No. 14-08-00505).

Experimental investigation of overequilibrium Xe atoms irradiation in shock waves propagating in He

Ziborov V S[@], Galiullin R A, Efremov V P and Fortov V E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vziborov@rambler.ru

Shock tube study of noble gas mixtures Xe and He were done by multichannel emission spectroscopy at the end plate of shock tube. All measurements were carried out behind the incident shock waves at Mah number region 2.6 to 3.6. Spectrum region of interest was 200 to 750 nm. In addition the laser shliren method was used to meassure the dencity distribution in the shock wave front. Gas Xe was a small admixture to high purity He. The impurity gas concentration was less 0.0001%. The regims of shock waves propagation in which Xe irradiation lines were observed at the lokal hot areas on shock front surface were found. The investigation were supported by RAS.

A theory of pulsating and cellular detonations

Kasimov A R[1,@], Faria L M[2] and Rosales R R[2]

[1] King Abdullah University of Science and Technology, 4-2226, 4700 KAUST, Thuwal, Makkah 23955, Saudi Arabia

[2] Massachusetts Institute of Technology, Massachusetts Avenue 77, Cambridge, Massachusetts 02139, United States

[@] aslankasimov@gmail.com

Motivated by the success of the analog model of pulsating detonations developed in [1, 2], we have developed an asymptotic theory of weakly nonlinear multi-dimensional detonation waves. Neglecting dissipative effects, we obtain the following (non-dimensional) system of equations [3]:

$$\begin{aligned} u_t + uu_x + v_y &= -\frac{1}{2}\lambda_x, \\ v_x &= u_y, \\ \lambda_x &= -k(1-\lambda)e^{\theta(u+q\lambda)}, \end{aligned}$$

where (u, v) is the velocity field, $\lambda \in [0.1]$ is the variable measuring the fraction of the total chemical energy, q, released in the reactions, k is the pre-exponential factor, and θ is the effective activation energy. The first equation in the system is seen to be a 2D Burgers equation forced by the chemical energy release, the second is the condition of zero vorticity, and the third is the equation of kinetics. Numerical computations with the model show that it can predict cellular detonations in 2D as well as pulsating detonations in 1D in precise agreement with numerical simulations of the full system of the reactive Euler equations.

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The formation of ignition centers before the front of spherical flame of hydrogen–air mixtures under intense initiation

Petukhov V A[@], Bublik N P, Gusev P A, Gutkin L D and Solntsev O I

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] petukhov@ihed.ras.ru

In studies of evolution of spherical hydrogen–air flame at various energies of initiation it has been found formation of ignition centers before the primary flame front. Combustion mixture was enclosed into thin rubber envelope having spherical shape and the initial volume of up to 40 m^3, which was located in the spherical explosion chamber 13YA3 12 m in diameter. At initiation energy 2.3 kJ ignition centers occur in a stoichiometric mixture in the initial volume of 40 m^3. In the stoichiometric mixtures and the poorer ones in the volume of 7 m^3 at the same initiation energy no ignition centers occur. In the volume of 7 m^3 in the stoichiometric mixtures ignition centers occur with increasing of initiation energy up to 4.6 kJ. With increasing of initiation energy up to 15.5 kJ in the volume of 7 m^3 ignition centers occur in the mixtures of 24 vol. % H_2 and richer. Up to this study the ignition of hydrogen–air mixtures are observed only after reflection of shock waves from flat and concave reflectors. In the spherical flames such phenomena are observed for the first time. The reason of occurring of ignition centers is gas heating before the combustion front to auto-ignition temperature at the cost of passing of the primary shock wave and waves generated by the expanding flame front. Thus, at increasing the initial volume of the hydrogen–air mixture, energy initiation at which the ignition centers occur before the primary flame front, decreases. The result is important for the analysis of emergency hydrogen explosions at industrial sites, such as nuclear power plants.

Numerical and experimental analysis of propane–hydrogen mixture ignition in air

Sevrouk K L[1,@], Krivosheyev P N[1], Penyazkov O G[1], Torohov S A[2], Titova N S[2] and Starik A M[2]

[1] Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus, P Brovka Street 15, Minsk 220072, Belarus
[2] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

[@] sevrouk@dnp.itmo.by

The addition of hydrogen to the various hydrocarbon fuels being examined as a promising method for increasing the efficiency of the engine while improving their emission characteristics. At the literature, researchers extensively studied effects of the addition of hydrogen at the time of ignition, flame velocity and flame stability, changes in the concentration of hazardous substances in the combustion products. For example, it was shown experimentally that the addition of hydrogen to methane significantly reduces the ignition delay time in the range of initial temperature 1–2 kK and a pressure 5–20 bar. A similar tendency was registered by the addition of H_2 to a mixture of 92% methane and 8% ethane at temperature 0.9–18 kK and pressure 1–16 bar, as well as to propane at temperature 1–1.6 kK and pressure 1.2–10 bar. Investigations of ignition delay time changes with the addition of hydrogen to heavier hydrocarbons (heptane, i-octane, n-decane) is carried out only on the basis of numerical simulation. The presence of a negative temperature coefficient according to saturated hydrocarbons C_nH_{2n+2} ($n \geqslant 3$) leads to the following characteristics: at relatively high temperature 1–1.6 kK the hydrogen additive accelerates ignition and at a low temperature—slows down.

The aim of this work is to messure the ignition delay time C_3H_8–H_2 mixture in the air and analysis of the mechanisms responsible for the acceleration of chain reactions with the addition of hydrogen in propane, based on numerical simulation.

The influence of coal particles on self-ignition of methane–air mixture at the temperature 950–1200 K

Leschevich V V, Penyazkov O G, Shimchenko S Yu[@] and Yaumenchykau M L

Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus, P Brovka Street 15, Minsk 220072, Belarus

[@] sergey.shimchenko@gmail.com

This paper represents experimental investigation of ignition of combustible gaseous mixture with reactive particles in the rapid compression machine at temperature 950–1200 K and pressures 1.5–2.0 MPa. The experiments were carried out with stoichiometric methane–air mixture in the presence of coal particles at size 32 μm. It was found that the presence of these particles not only reduces ignition time but influences on the ignition temperature of mixture. It is ascertained that ignition time of methane in pure air is longer than with same mixture with addition coal dust. This difference is explained to preignition of methane near burning particles. It is shown that ignition of coal dust originates at the temperature of oxidant higher 850 K. Temperature of particles burning in methane–air and air environment heated by compression was measured. The mean temperature is 2500 K. It indicates possibility of premature ignition of gas mixture heated by compression to temperature 1000–1100 K by addition of coal particles.

Luminescent characteristics of the shock-wave ignition of an ethylene–oxygen mixture

Smirnov V N[1,@], Tereza A M[1], Vlasov P A[1,2], Shumova V V[3,1], Garmash A A[2] and Demidenko T S[2]

[1] Semenov Institute of Chemical Physics of the Russian Academy of Sciences, Kosygina 4, Moscow 119991, Russia
[2] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[3] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vns1951@yandex.ru

The ignition of a stoichiometric ethylene–oxygen mixture diluted with argon was studied experimentally and computationally to gain new insights into the nature of the chemiluminescence that accompanies this process and to obtain some of its quantitative characteristics. The experiments were performed behind reflected shock waves at temperatures of 1270–1820 K and a pressure of $\sim$ 1 bar. The time evolution of the intensity of the luminescence of electronically excited radicals C_2^*, CH^*, and OH^* and molecule CO_2^* was monitored photometrically. The measured temperature dependence of the ignition delay time was found to be in close agreement with the published data and the results of simulations within the framework of the ChemphysMech_v.1 reaction mechanism. An analysis of the possible reactions of formation of C_2^*, CH^*, and OH^* and molecule CO_2^* was carried out. It was for the first time shown that, along with the recombination reaction $CO + O \rightarrow CO_2^*$, CO_2^* is formed by the reaction $CH + O_2 \rightarrow CO_2^* + H$, which, moreover, dominates during fuel burnout, whereas the former becomes dominant later, in the post-combustion recombination stage. The contribution from the reaction $C_2H + O_2$ was demonstrated to play a minor role in the formation of CH^* as compared to the $C_2H + O$ reaction, at least under the conditions tested.

Ignition delays in methane–oxygen mixtures in the presence of small amount of iron or carbon nanoparticles

Eremin A V[@] and Gurentsov E V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] eremin@ihed.ras.ru

The influence of small additions (0.3–2 ppm) of iron or carbon nanoparticles on ignition delay times of stoichiometric 20% methane-oxygen mixture in argon was investigated. The experiments were performed in 50 mm diameter shock tube behind reflected shock waves. The nanoparticles were synthesized in the experiment before the ignition test in pyrolysis of 0.5–1% of $Fe(CO)_5$ and of 1–2% of C_6H_6 diluted by argon. The residual nanoparticles entered in the flow behind incident and reflected shock wave from the shock tube walls and their volume fraction was measured by laser light extinction at the wavelength 633 nm. Additions of 0.3–2 ppm of iron nanoparticles to stoichiometric methane–oxygen mixture resulted in the twofold decrease of ignition delays at temperatures below 1400 K relatively to calculated and experimental data for the mixture without nanoparticle addition. At additions of 0.4–1 ppm of carbon nanoparticles to stoichiometric methane-oxygen mixture a weak ignition delay decrease relatively to the calculated data for the mixture without additives of carbon nanoparticles was observed.
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Influence of hydrogen, methane and syn-gas additives on acetylene detonation

Drakon A V, Eremin A V, Kiverin A D and Tsirlina E A[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] elena2509@yandex.ru

In the present study the analysis of possibility of initiation of oxygen-free detonation wave of condensation in the model mixtures $6\%C_2H_2$ + Ar, $6\%C_2H_2$ + $50\%H_2$ + Ar and $6\%C_2H_2$ + $50\%H_2$ + $6\%CH_4$ + $32\%CO$ + $6\%CO_2$, the reflecting an average structure of gas products of oxidizing pyrolysis of methane, was carried out.
Modeling was carried out in a software package of ChemKin and in an original package [1]. The kinetic mechanisms [2, 3], describing thermal decomposition of acetylene and formation of carbon nanoparticles and also the GRI-Mech 3.0, allowing description of the thermal decomposition of methane and interaction of CO and CO_2 with products of pyrolysis of methane and acetylene, were used. Calculations were carried out in zero-dimensional isobaric approach (without gasdynamic effects). The initial temperatures of mixture were varied in the range of 1200–2000 K; the values of pressure of 6 and 30 bar close to conditions of experimental work [4] were used.
Performed calculations have shown that in the considered mixtures the process of condensation and heat release is delayed relatively to acetylene without additives up to two orders of magnitude that allows to draw a conclusion that attempts to initiate a detonation wave of condensation in similar mixtures look unpromising.

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Attenuation of the detonaiton wave in hydrogen–air mixture

Bivol G Yu[@], Golovastov S V and Golub V V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] grigorij-bivol@yandex.ru

Detonation propagation in undiluted hydrogen-air mixture in acoustically absorbing channel at atmospheric pressure was investigated experimentally. Since the detonation wave has a cellular structure, one of the ways to prevent the detonation could be to use particular forms of coating, to diminish the intensity of transverse perturbations [1]. The goal of this work was to determine of the parameters of the detonation wave in hydrogen–air mixtures with the acoustically-absorbing coatings with open pores. The parameters were determined in dependence on the hydrogen concentration and the thickness of the absorbing layer. Inner walls of a part of the channel were covered with an acoustically absorbing material. Experiments were carried out in undiluted mixture at atmospheric pressure. Detonation was formed as a result of a deflagration to detonation transition. Ignition of the hydrogen-air mixture was carried out by a spark gap at a closed end of the detonation tube. A stationary detonation wave was formed before the entering the absorbing section wit the acoustically adsorbing walls. After passing the absorbing section parameters of the detonation/shock wave were measured. It was found that the recovery of the detonation wave can occur after the absorbing section.

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Deflagration to detonation transition in curved channels

Mikushkin A Y[@] and Golovastov S V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] mikushkin-anton@yandex.ru

There are a lot of ways of reducing the transition of combustion to detonation. One of them is the use of various types of geometrical barriers set inside the channel through which propagates a flame front: a ring of barriers [1], spirals [2], etc. Due to the reflection of wave perturbations, propagating in front of an accelerating flame front, form additional foci of ignition. This leads to additional energy release and the reduction of predetonation distance. Also the obstacles lead to a decrease in impulse of the combustion products. The aim of this work was experimental determination of the dynamics of transition of combustion into detonation within a channel arranged inside the flat spirals in hydrogen–air mixtures.

Experiments performed for three values of ER (equivalence ratio) of 0.7, 1.0 and 1.5, showed that the formation of detonation when using spiral plate occurs on the first turn of the spiral used for all three values of ER. The comparison of experimental data obtained using a flat plate showed that the observed effect is due solely to the curvature of the surface, and not a decrease in the effective diameter compared to the diameter of not separated initial channel. Thus, the use of spirals can be an effective element to reduce the predetonation distance.

The work was supported by the Russian science Foundation (No. 14-50-00124).

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Theory and experiments of premixed turbulent combustion

Krikunova A I[@] and Son E E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] utro-2007@mail.ru

Turbulent combustion is the one of the most important unsolved problems in modern science. Based on the probability density function, a model of turbulent combustion can be developed. The system of Reynolds equations describing the behavior turbulent flows is not closed, and usually for the numerical simulation is used some mathematical models. However, each model has limits of application. But as known, the probability density function allows to calculate the statistical moments of any order. And then approximate models are no more need. Thus, the description of turbulent flow is brought to the experimental finding of joint probability density functions, such as speed and concentration. To reduce the system of Reynolds equations, it is worthwhile to simplify conditions: premixed flame suspends interdiffusion of fuel and oxidizer, and microgravity conditions remove buoyancy forces, that in its terms have significant influence on flame properties and behavior. Hence the most appropriate object for investigation and to deep insight fundamentals of turbulent combustion are conical premixed flames in reduced gravity. In previous works was detailed investigated behavior of diffusion flames under microgravity conditions, and premixed V-shaped flames. A lot of properties and laws were derived, such as flammability limits, burning velocity, minimum ignition energy, flame height, flame velocity and its pulsation, and some others. Despite on all of this investigations unfortunately was not developed universal model of turbulent combustion and this issue is still open and future investigation could help to make significant steps in this direction.

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Acoustic control of the structure of the gas torch

Golub V V[@], Krivokorytov M S and Volodin V V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] victor.v.golub@gmail.com

Diffusion torches have studied experimentally in the transverse acoustic field. The structure and the luminosity of a torch have recorded by a high-speed camera with shadow device and photodetectors. The dependence of the length of a laminar methane plume on the average velocity and volumetric flow rate have obtained and compared with the classical ideas about the length of laminar flames. The frequency spectra of the luminosity of the flame at different flow rates of methane have obtained. Flame flicker frequency depending on the volume flow of methane have defined according to the obtained spectra. It was found that the flame flicker frequency is not dependent on the diameter of the burner. It is shown that the flicker are caused by changes in the geometric dimensions of the flame due to the convective instability of the column of hot gas surrounding the torch. The repetition frequency of the vortices in the column of hot gas surrounding the torch coincides with the frequency of the flicker of the flame.

It is shown that the limit of flame detachment from burner does not change at the acoustic impact on the torch, the biggest acoustic impact has on the contrary attaching detached torch. Fuel speed range, in which there is detached steady torch, increases.

The work was supported by the Combustion and Explosion Program of RAS Presidium.

Flame front propagation in a channel with porous walls

Bivol G Yu[@], Golovastov S V and Golub V V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] grigorij-bivol@yandex.ru

Decay and deceleration of a detonation wave was experimentally studied in a rectangular channel for hydrogen-air mixtures. Inner walls of a part of the channel were covered with an acoustically adsorbing wall. Experiments were carried out in undiluted mixture at atmospheric pressure. Preliminary the detonation was formed as a result of a deflagration to detonation transition. Ignition of the hydrogen-air mixture was carried out by a spark gap at a closed end of the detonation tube. The second end of the tube was opened. A stationary detonation wave was formed before the entering the absorbing section wit the acoustically adsorbing wall. Dynamics of the flame were recorded using a high-speed camera. It was observed, that the flame has a V-shaped profile in acoustically adsorbing section. The streak-image of the dynamics of the flame front and detonation products along the axis of the channel was observed. It was supposed that the shape of the flame is caused by an additional heating the hydrogen-air mixture in open pores by initial shock wave or an acceleration of the flame front along the boundary due to a friction.

The work was supported by the Russian Science Foundation, grant No. 14-50-00124.

Analysis of thermodynamic parameters behind detonation wave front in hydrogen–air mixtures on base of streak-images

Samoilova A A[1], Bivol G Yu[2] and Golovastov S V[2,@]

[1] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] golovastov@yandex.ru

During numerical simulations of detonation wave propagation in gas mixtures an initial mechanical and thermodynamic condition of the gas products behind the front of the detonation wave is often taken into account. This especially concerns the problems in which the motion of the gas behind the front has a major contribution to the phenomenon under investigation.

Evaluation of the thermodynamic parameters of the combustion products of the detonation of stoichiometric hydrogen-air mixture behind the detonation front was carried out in the adiabatic expansion of the detonation products with "frozen" the composition and taking into account the changes of the equilibrium composition on the base on trajectories of glowing combustion products. The velocity of the combustion products and their trajectory are determined based on the streak-images obtained via self-luminosity of hot detonation products. The front of the detonation wave was considered as an ideal chemical reactor that transforms the initial equilibrium thermodynamic state for the final equilibrium thermodynamic state. It is shown that in the case of the adiabatic approximation thermodynamic parameters can be approximated by a polynomial of the second degree. Conversely, the chemical conversion leads to the temperature reduction up to 3–15% in comparison with the adiabatic approximation.

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Reflected acoustic wave impact on frame front acceleration

Korobov A E[@] and Volodin V V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] andrusha.kor@gmail.com

The frame front velocity during deflagration of air-hydrogen mixtures strongly depends on the instability of the frame front. Effect of the acoustic field on the phase of the energy release phase and thermodynamic parameters of burning gas is given in [1] for the deflagration to detonation transition, in [2] for combustion. In [3, 4], the character of the impact of the acoustic field on the jet of fuel mixture and further combustion of the jet is described. Despite the fact that the generated external acoustic field may be a promoter, that accelerates the flame front, an analogous acoustic field may also lead to the destruction of the instabilities when the field intensity exceeds the intensity of the generated instabilities, and frequency or the phase are without resonate. A similar method may be effective in preventing of the development of dangerous combustion modes. The aim of the work was to determine the frequency spectrum of the acoustic disturbances that are emitted by the accelerating flame front in a hydrogen-air mixture and the effect of acoustically absorbing coatings on the velocity of the flame front. This work was supported by the Russian Science Foundation, grant No. 14-50-00124.

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Flame propagation in transient turbulent flow fields

Medvedev S P[@], Khomik S V, Maximova O G, Agafonov G L, Mikhalkin V N and Betev A S

Semenov Institute of Chemical Physics of the Russian Academy of Sciences, Kosygina 4, Moscow 119991, Russia

[@] s_p_medvedev@chph.ras.ru

Combustion in burners, engines, furnaces, and fires generally occurs via turbulent flame propagation. Fundamental properties of turbulent flames are usually studied under steady turbulent flow conditions. A well-known example is homogeneous isotropic turbulence generated in a fan-stirred combustion bomb. An opposite example is that of transient turbulence in reciprocating engines. Experimental study of flame propagation in a transient turbulent flow field (TTFF) can elucidate characteristics of practical combustion systems that cannot be examined by conventional techniques. The following techniques are proposed and tested in this work: (1) TTFF generation by a short-duration compression pulse; (2) TTFF generation by sudden expansion; (3) TTFF generation in a shock tube under over-tailored conditions. A common advantage of these techniques is the use of a laboratory shock tube. Experiments were performed in a 25 mm square shock tube and a cylindrical explosion chamber of 120 mm in diameter. It was found that turbulent fluctuation velocity can be varied over a wide range up to 10 m/s. Application of the proposed techniques to the study of flame propagation at autoignition conditions is discussed. Another prospective area of research is turbulent flame propagation in a gas containing micro-droplets produced by sudden expansion.

On the exothermal reaction kernel formation in shock tube

Kiverin A D[@] and Yakovenko I S

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] alexeykiverin@gmail.com

According to the ideal shock tube theory the induction stage takes place at constant temperature and pressure in the adiabatically compressed mixture behind reflected shock. However in case of low reactivity one can observe localized ignition inside kernels. For the first time such a regime of ignition was observed by R I Soloukhin and further was systematically observed in shock tubes. According to [1] the scenario with formation of ignition kernels and sequential mixture burning in flame regime fully determines the distinctions between kinetic calculations and experimental data at low temperatures. Thus the basic question to get full understanding of the "mild ignition" phenomenon concerns the origins of these ignition kernels. The results of this paper based on 3-D simulations of the flow evolution behind the incident and reflected shocks allow formulation of the following scenario of ignition kernels formation. Initial stage during and after the diaphragm rupture is characterized by a set of non-steady gasdynamical processes. As a result the flow behind the incident shock occurs to be saturated with temperature perturbations. Further evolution of these perturbations provides generating of the shear stresses in the flow accompanied with intensification of velocity and temperature perturbations. After reflection the shock wave interacts with formed kernels of higher temperature and more pronounced kernels arise on the background of reactivity profile determined by moving reflected shock. Exothermal reaction starts inside such kernels and propagates into the ambient medium via spontaneous ignition wave with minimum initial speed equal to the shock wave speed.

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Peculiarities of numerical analysis of unsteady reactive flows

Yakovenko I S[@], Kiverin A D, Ivanov M F and Pinevich S G

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] yakovenko.ivan@bk.ru

Numerical modeling is one of the most effective techniques for theoretical analysis of fundamental and applied problems of combustion and detonation physics. However the problem of choosing a proper numerical approach for modeling the process of unsteady reactive flows evolution on the large time scales and on precise three-dimensional numerical grids is still controversial. Present study discusses capabilities of dissipation-free CABARET numerical method application to unsteady reactive gasdynamic flows modeling. CABARET numerical method was fully developed and described in series of papers by Goloviznin *et al* [1,2]. In framework of present research it was adopted for reactive flows governed by real gas equation of state and applied for several typical problems of unsteady gas dynamics and combustion modeling such as ignition and detonation initiation by localized energy sources. Solutions were thoroughly analyzed and compared with that derived by modified Euler–Lagrange method of "coarse" particles (CPM) described in [3] and intensively used by authors in their previous studies [4]. Obtained results allowed us to distinguish range of phenomena where artificial effects of numerical approach may counterfeit their physical nature and to develop guidelines for numerical approach selection appropriate for unsteady reactive gasdynamic flows numerical modeling.

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Combustion onset in channels induced by hydrogen jet propagating from the high pressure chamber

Golub V V, Golovastov S V, Ivanov M F, Kiverin A D and Smygalina A E[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] anna.smygalina@gmail.com

The ever-growing tendency of hydrogen utilization as a fuel for advanced engines made the problem of save hydrogen storage currently important. In a number of numerical as well as experimental studies it was shown that when hydrogen jet propagates from the high pressure chamber into the air the selfignition of hydrogen mixed with air behind the shock wave occurs at certain nozzle diameter, hydrogen pressure, channel length and diameter. In the majority of experiments initial pressures in the driver section were chosen higher than 10 MPa what guaranteed selfignition occurrence but did not define low limits of pressure for selfinition. In the present investigation experiments were carried out at relatively low pressures of hydrogen in driver section and normal pressure of air in driven section and it was demonstrated that selfignition occurs even at hydrogen pressure of 6 MPa. Mathematical modelling with the task options close to the conditions of experiments enabled to scrutinize the process. In the performed calculations as in the experiments selfignition emerged near the channel walls and the timing of ignition both in mathematical and physical experiments was almost the same, 90-94 us. Both computational and experimental results showed that the selfignition timing substantially depends on the diaphragm rupture timing. The selfignition timing rises along with the rupture timing so when the latter is greater than 110 us the selfignition does not occur.

Experimental and computational procedures for investigation of methane–hydrogen combustion in spark ignition engine

Zaichenko V M, Ivanov M F, Kiverin A D, Smygalina A E[@] and Tsyplakov A I

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] anna.smygalina@gmail.com

One of the most perspective strategies in the modern energetics is the utilization of hydrogen and methane–hydrogen mixtures in spark ignition (SI) engines. In the present work, the installation for experimental investigation of methane–hydrogen combustion in dedicated internal combustion engine G-266 was developed. Engine G-266 represents the 6-cylinder diesel engine D-266.4 converted on gaseous fuel. Displaced cylinder volume is 1.187 l, compression ratio—11.0, rotational speed—1500 rpm. The facility features the use of hydrogen-containing mixtures characterized by low detonation stability, thus, the supercharging system was excluded while intaking system was transformed. The engine is supplied by the microprocessor spark timing and rotational speed controlling systems. In order to test the elaborated installation experiments were performed with the use of stoichiometric methane–air mixture at full and part loads (48 and 37 kW); with and without spark ignition. Computational experiments of combustion in SI engine were carried out as well. The mathematical model represents the Navier–Stokes gasdynamic system of equations with account of molecular transport processes. The chemical transformation is described by reduced kinetic mechanism. Obtained computational indicator diagrams gave a good correspondence with experimental ones. This result may be esteemed as a confirmation of computational technique reliability, which is important in order to perform further predictive computations prior to experiments with hydrogen-containing mixtures.

Shock wave in combustible gas containing a microparticle

Efremov V P, Obruchkova L R[@], Ivanov M F and Kiverin A D

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] o_liliya@ihed.ras.ru

Influence of inert firm particles on initiation of detonation of combustible gases is located in focus of modern detonation physics. The urgency of such a problem is caused by requirement of catastrophic explosions prevention. For example such research is important for justification of safety of the nuclear power plants. A two-dimensional hydrodynamic code is used to simulate shock wave in a tube, which initially consists of two chambers. Chambers are separated by the membrane. The membrane is removed instantaneous. The code [1] allows carrying out study of burning and combustion processes in combustible gases. It is known, that before nonmoving particle the heat energy is generated by gas flow stopping. In the present work the progress of the detonation initiation due to additional heat generation is considered. The wall of tube is supposed to be adiabatic. The particle is assumed to be nonmoving, thermal nonconductive and chemically non-reacting. Despite of many limitations this approach can be used to our case and allows analyzing time of induction nearby after the shock wave front. It is shown, that velocity and temperature relaxation times are much more than time interval between shock wave and rarefaction wave arrivals to the particle. It is shown, that presence of the microparticle can change time of induction.

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Experience on math simulation of aerogasdynamic and shock wave processes accumulated by the State Rocket Centre

Degtiar V G and Khlybov V I[@]

Open Joint Stock Company "Academician Makeyev State Rocket Centre", Turgoyakskoye Shosse 1, Miass, Chelyabinsk Region 456300, Russia

[@] vik_20152016@mail.ru

In the field of aerogasdynamics and heat exchange math and simulation models are based on software with Navier–Stokes equations describing the movement in continua (CFD packages) or direct statistic modelling to solve Boltzmann equations for movement in rarefied medium. The paper gives consideration to experience in using supercomputer simulation modelling of aerogasdynamics and heat exchange, when designing items of space rocketry. The paper covers issues of numerical simulation of processes:

(i) at launch, including air launch of a launch vehicle (LV) from a carrier aircraft; vertical and horizontal underwater launch; design and experimental study of gasdynamics of exhaust streams from a cluster of nozzles and processes of ejection in gaps of a launcher;

(ii) in flight, including flight in continua at sub- and supersonic velocities up to 70–80 km and separation of LV stages; design and experimental study of a flow pattern at the bottom of a supersonic LV flying at a supersonic velocity in rarefied medium up to 150 km;

(iii) interaction of shock waves with an LV flown at an altitude at a supersonic velocity.

There are math simulation models for each problem that permits getting not only integral and distributed parameters of interaction with environment at a design accuracy and studying physical processes outside and inside complicated configurations but also optimizing the system configuration and operation modes, if needed.

Central-upwind schemes for numerical simulation of shock wave processes in layered media

Khlybov V I[1,2] and Pridannikov A V[1,@]

[1] Open Joint Stock Company "Academician Makeyev State Rocket Centre", Turgoyakskoye Shosse 1, Miass, Chelyabinsk Region 456300, Russia
[2] South Ural Scientific Centre of the Ural Branch of the Russian Academy of Sciences, Oktyabrya Avenue 16, Miass, Chelabinsk Region 456318, Russia

[@] bugs001@mail.ru

The necessity to simulate shock wave processes in layered media appears in problems of a physics of an explosion and when studying interactions of intensive radiant (particle) fluxes with substance. At present upwind schemes are widely used to numerically simulate processes in mechanics of continua with discontinuous solutions (shock waves or contact discontinuities). In so doing, the application of the methods for complex equations of state is a rather nontrivial task and asks for considerable computational efforts.
An alternative approach to upwinding is based on the use of centered approximation which leads to central schemes. Their key advantage as against the above mentioned methods is no need in Riemann solvers (which are physics-specific).
When central schemes are used to simulate processes with contact discontinuity, there occurs a problem of a so-called "mixed cell" in a place of contact. This work deals with the application of a central-upwind scheme for simulation of 1D shock wave processes in layered media. We propose an algorithm to compute parameters in contact discontinuity that lies in the application of Kuropatenko's method, when a shock wave passes through the contact. When a rarefaction wave passes by, special projection procedure is implemented. It should be noted that the proposed algorithm imposes no limits on a type of equations of state. Test runs were performed for 1D environment and proved that the proposed algorithm did not yield to available upwind schemes in accuracy and had less computational efforts for complex equations of state.

Influence of a dispersed phase presented in external flow on heat exchange and erosion damage of surface of a hypersonic flight vehicle

Merkulov E S[1,2,@] and Lepikhov A V[1,2]

[1] Open Joint Stock Company "Academician Makeyev State Rocket Centre", Turgoyakskoye Shosse 1, Miass, Chelyabinsk Region 456300, Russia
[2] South Ural Scientific Centre of the Ural Branch of the Russian Academy of Sciences, Oktyabrya Avenue 16, Miass, Chelabinsk Region 456318, Russia

[@] mes1@yandex.ru

It is well known that our planetary atmosphere has a complex set of components, including water vapors, which tend to condense into a droplet phase particularly at altitudes of 2–13 km above the Earth's surface. Hence, a flight vehicle (FV) may fly in turbulent multiphase polydisperse nonequilibrium environment with high probability. In so doing the surface of hypersonic FVs is exposed to heavy thermal loads, even in free flow. The droplet phase presented in the flow can change the FV thermal conditions. The paper is devoted to passing of the droplet phase through the hypersonic FV bow shock wave. We consider splitting of droplets, when they pass through a shock wave and their evaporation in high-enthalpy flow over the FV.
We present a methodology for numerical simulation of the interaction of the dispersed flow with the supersonic FV. The methodology is based on Navier–Stokes equations that account for a Lagrange phase presented in flow. We make an assumption that particles and free flow may interface with each other. The particles can collide with one another and break up. We take into account the water evaporation from surface of particles which leads to increase in concentration of water vapor in an area adjacent to the FV. We made test runs using the described model. We made a conclusion on the influence of dropping liquid presented in flow on a flow pattern and heat exchange over the supersonic FV surface. We consider the possibility of erosion damage of the surface thermal protection effected by the dispersed phase.

CABARET numerical scheme implementation for the viscosity-stratified fluid flows

Kulikov Yu M[@] and Son E E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] kulikov-yurii@yandex.ru

Computer performance intensive raise impacts significantly on the CFD while the actual speed in solving applied problems also depends on the program algorithm efficiency and the quality of the numerical methods. The CABARET numerical scheme represents a new approach to the convective fluxes approximation in problems dominated by transport phenomena including shock-wave propagation, aeroacoustics, swirling and turbulent flows, as well as those in which the transport coefficients (viscosity, thermal conductivity, electrical conductivity) are abrupt functions of thermodynamic potentials eigenvariables. Often being non-monotonic such substantial coefficient variation can be a consequence of chemical reactions and phase transformations.

In present paper the Cabaret scheme has been implemented for Riemann problem. Simulation results confirmed this scheme to be an effective tool for discontinuous flows modeling along with weak dissipative properties. We used barotropic equation of state $p = c^2(\rho - \rho_0)$ where c and ρ_0 stands for the sound velocity and density of water under normal conditions. Basing the results of one-dimensional testing we have implemented algorithm for calculating three-dimensional viscous liquid flow in a rectangular channel with several types of boundary conditions. We tested the mesh transfer along different spatial directions in the problem of isothermal and non-isothermal channel viscous flow and also simulated the entry flow of thermoviscous fluid in strongly inhomogeneous temperature field.

The work was supported by the Russian Science Foundation project ID 14-50-00124.

Calculations of scaled model of the HEXAFLY-CIAM module in FlowVision software

Markova T V[1,@], Aksenov A A[1], Gavrilov A D[1], Prokhorov A N[1,2], Son E E[1], Zhluktov S V[1] and Savitsky D V[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

[@] markova@flowvision.ru

A prospective hypersonic HEXAFLY aircraft is considered in the given paper. In order to obtain the aerodynamic characteristics of a new construction design of the aircraft, experiments with a scaled model have been carried out in a wind tunnel under different conditions. The runs have been performed at different angles of attack with and without hydrogen combustion in the scaled propulsion engine. Numerical simulation allows one to reduce the number of wind tunnel experiments as well as to obtain aerodynamic characteristics for any possible design of the full-scale aircraft under different operation conditions. Therefore it is important to have a reliable CFD software. The reliability of the numerical predictions must be confirmed in verification study of the software. The given work is aimed at numerical investigation of the flowfield around and inside the scaled model of the HEXAFLY-CIAM module under wind tunnel conditions. A cold run (without combustion) is considered. The calculations are performed in the FlowVision software. The flow characteristics are compared against the available experimental data. The carried out verification study confirms the capability of the FlowVision software to calculate the flows discussed. Therefore, the software can be used for calculations of the aerodynamic characteristics of the scaled and full-scale models of the vehicle under different operation conditions. This work was supported by the Ministry of Education and Science grant No. 14.604.21.0090, project ID: RFMEFI60414X0090.

Numerical study of high-speed civil aircraft HEXAFLY-INT large-scale model intake characteristics

Gouskov O V[1], Danilov M K[1,@], Kukshinov N V[1,2] and Rudinskiy A V[1]

[1] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] danilovm@ciam.ru

Numerical study of intake characteristics of high-speed civil aircraft HEXAFLY-INT (high speed experimental fly vehicles–international) was carried out in the work. In high-speed aircraft concept proposed by European Space Agency within the scope of international cooperation project HEXAFLY-INT the intake has a complex 3D configuration. After assessment of cost and time of the intake producing it was decided for the first phase of work to produce simplified technological intake. The technological intake has three compression ramps and provide similar flow characteristics in the inlet of internal flowpath. Comparing calculations of original and technological intakes were performed with the same free stream parameters. The comparison of two intakes was made on the throat flow parameters. The good correspondence of results was obtained. Further the intake start in flight conditions corresponding to Mach numbers M = 4–8 was calculated. The flight regimes corresponding to started and unstarted intake were defined. The flow parameters in the throat were defined. The calculations were carried out within numerical solution of averaged full Navier–Stokes equations with the aid of code developed in CIAM.

The investigation of work process in combustor of high-speed civil aircraft HEXAFLY-INT large-scale model

Batura S N[1] **and Kukshinov N V**[1,2,@]

[1] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] kukshinov@ciam.ru

In the paper the combustion of hydrogen-air mixture in the combustor of high-speed civil aircraft HEXAFLY-INT (high speed experimental fly vehicles–international) large-scale model was investigated. The internal duct has elliptical configuration and was designed for providing combustion in supersonic flow. Hydrogen was used as the fuel. The fuel injection is divided in 2 stages. The calculation was carried out in 3D definition with turbulence model and detailed chemical kinetics mechanism. The calculation was performed within solution of RANS equations for unsteady turbulent flows. For hydrogen-air mixture combustion calculation the Dimitrow detailed chemical mechanism was used. The calculated geometry model represents the internal duct integrated with the intake. Such problem definition allows to obtain fields of gasdynamic parameters in the combustor inlet with account for complex gasdynamic structure affecting to ignition and combustion processes. As the result the distributions of flow parameters along the combustion chamber were obtained. The evaluation of combustion efficiency was performed. The comparison with experimental data obtained in HEXAFLY-INT large-scale model tests in CIAM test facility was performed.

Numerical simulation of hydrogen pulse combustion regime in high-velocity flow

Batura S N[@] and Gouskov O V

Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

[@] since85@mail.ru

The paper is dedicated to numerical simulation of pulse combustion regime of supersonic hydrogen–air mixture. Pulse operating regime of a combustion chamber makes enquires into the possibility of a new ramjet scheme development, in which combustion takes place in a pulse wave structure of a pseudoshock type and average velocity in a duct close to transonic. Such a workflow is assumed to achieve more effective fuel combustion as compared to combustion in a supersonic flow. P K Tretyakov and his team from the Institute of Theoretical and Applied Mechanics SB RAS have been studied this problem for many years. Their papers describe different variants of the combustion chamber design and types of energy influence on a flow when combustion process is pulse. In this work a valve system with air pulse generator is used to influence the flow. The air is supplied in the constant cross-section area perpendicular to the main flow direction. For numerical calculation used set of computer programs FNAS 3D, developed in CIAM. This program is based on the procedure for finding time steady-state solution using S K Godunov numerical scheme. A full set of Favre-averaged Navier–Stokes equations for unsteady turbulent reacting flows uses in the program. To describe the combustion of hydrogen–air mixture using a Dimitrov's detailed kinetic mechanism. The calculation shows the feasibility of flow realization similar to the flow observed in the experiment. The comparison of pressure distribution on the wall of the channel was carried out.

Hypersonic and plasma technologies development in the Moscow Institute of Physics and Technology

Prokhorov A N[1,@], Son E E[3], Arefyev K Yu[1,2] and Son K E[3]

[1] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia
[3] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] prokhorov@ciam.ru

Since 2014 a new development stage of hypersonic and plasma technologies (HaPT) has started. From the year of HaPT foundation till nowadays fundamental, exploratory and applied experiment-calculated research in the field of perspective hypersonic aircrafts design have been made. Physical laws of high-velocity and high-enthalpy single- and two-phase medium have been explored. Within the framework of HEXAFLY-INT project on civil high-velocity aircraft creation, the Moscow Institute of Physics and Technology (MIPT) laboratory has carried out the numerical modeling of scaled model with FlowVision software package in flight and ground test conditions. In 2015 unique spectral measurements of plasma were carried out. Probing devices of high-melting materials, processing systems and interpretation models of the probing devices output signals were designed and created. Model experiments with probes in the high temperature jet of plasma torch in a temperature range from 5000 to 10000 K were carried out. The studies and the obtained results allowed strengthening MIPT cooperation with scientific and industrial partners, as well as other research institutions and industrial enterprises. Currently available MIPT technological advance in the field of hypersonic and plasma technologies corresponds to the world standards and will to be used for the thematic works, as well as fundamental and applied research.

Interaction of entropy and acoustic waves in combustion chambers of high-enthalpy air flow generators

Aleksandrov V Yu, Arefyev K Yu[@], Ilchenko M A and Prokhorov A N

Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

[@] arefyev@ciam.ru

Creation of high-speed aircraft with air-breathing engine demands carrying out their ground tests in integration with propulsion. The generators of high-enthalpy air flows (HAFG) with vitiated heating and aerodynamic nozzles (ADN) with various extent of expansion can be used to carry out such tests and simulation of field environment. Use of HAFG demands the solution of a problem of working process stability in its combustion chamber (CC). It is experimentally established that in HAFG the high-frequency acoustic waves of pressure extending with a sound speed and low-frequency waves of entropy which speed of distribution is comparable with a stream speed in CC can exist. In the case under consideration waves of entropy appear owing to a variable heat supply in burning zone near injector head of CC caused by the changing ratio of components coming into CC. It is established that in case of an unstable regime of combustion the relative size of registered low-frequency temperature fluctuations caused by variable heating in a burning zone is significantly greater than relative fluctuations of temperature caused by pressure pulsations in isenthropic processes in CC.

The analysis of ramjet combustion chambers cooling conditions by means of polymeric compound gasification products

Arefyev K Yu[1,2], Fedotova K V[1,2,@] and Yanovskiy L S[1]

[1] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] wonnahrefn@icloud.com

The paper presents a mathematical model for the heat exchange dual problem in the combustion chamber with cooled walls of a high-speed ramjet engine on polymeric compounds as a fuel. This mathematical model takes into account the phase transformations of the polymeric compound gasification products within the cooling channels and nonequilibrium working medium flow in the combustion chamber duct. The basic structural parameters and allowable ramjet operating regimes were determined in terms of computational results analysis. Note that in this case permissible dimensions of the combustion chamber depend on air-to-fuel ratio and combustion products mass loading in the duct. At which time the regimes with less mass loading are attended by gasification products overheat. Higher values of mass loading cause the combustion chamber wall overheating. The basic requirements for polymeric compounds and their gasification products were developed. Advisory recommendations on high-speed ramjets validity range were worked out after the comparison of a number of polymeric compounds. Thrust estimation showed the effectiveness this fuel for various high-speed ramjets operation regimes. The obtained results can be used for the design of ramjet using polymeric compounds as a fuel.

Simulation of the combustion products cooling in the gas-dynamic channel of experimental facility by water injection

Abramov M A[1,2,@], Yakovchuk A Y[1], Fedotova K V[1] and Zaikin S V[1]

[1] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] abramovmaks94@gmail.com

Physical processes in the high-enthalpy experimental test facilities are investigated. The process of combustion products cooling by water injection into the gas-dynamic contour of the exhaust system is considered.
Water jet parameters, water droplets and gas heat and mass transfer processes, as well as droplets breakup and evaporation processes are calculated [1].
Ansys Fluent software is used for flow simulation and defining output parameters of the stream. To describe the motion of droplets in a continuous medium discrete phase model DPM (Discrete Phase Model) is used. The model based on the development of hydrodynamic instabilities on the droplet surface (Kelvin-Helmholtz and Rayleigh-Taylor) is activated for droplets breakup calculation [1].
The results give an idea of the physical process [2], and allow us to determine the following: required length of the cooling section, required water mass flow rate, gas flow temperature at the outlet, average water droplets diameter.
Gas-dynamic ducts in experimental facilities can be designed based on current paper results.

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High enthalpy flow generators for hypersonic wind tunnel facilities

Aleksandrov V Yu, Zaikin S V[@], Moseev D S and Yakovchuk A Y

Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

[@] Zaikin@ciam.ru

Different types of high enthalpy flow generators are used to model flight conditions while developing and testing hypersonic vehicles and engines. Each type of high enthalpy flow generators has some advantages and drawbacks, and therefore suits for its unique optimal application conditions.
Several types of high enthalpy flow generators are widely used:

- combustion heater,
- arc heater,
- cowper heater.

Review of high enthalpy flow generators, used in main hypersonic test facilities of USA, Japan, Europe and Russia, is presented in current paper. Test conditions, facility performance range, facility schemes and unique features has been compared. Cowper heater is presented in details. Different fillings heating processes and air heating in void passages between filling material are investigated computationally and experimentally.

Methods and ways to simulate real high enthalpy flight conditions for ground test facilities

Aleksandrov V Yu and Moseev D S[@]

Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

[@] dmitmoseev@yandex.ru

During test rig designing, one of the most important questions is the choice of method of working fluid heating, since the reliability of obtained results of engine test or high velocity aircraft test are related to that. There are three basic methods of air flow heating in the test rig duct up to demanded temperature, such as: heating of flow through a cowper device; electric arc heating; combustion heating.

The last method, undoubtedly, is most energy saving among considered those. However, before using this method, it should be a comparative analysis to determine, how much presence of impurities affects on the engine operation.

Modeling parameters of atmospheric flight at ground test facilities, which have combustion heating of a working body, bring about some difference of thermo-physical and chemical parameters for air and for simulating gas. This difference is caused by presence of pollutants (combustion products) in simulating gas. This situation causes, that complete simulation of hypersonic flight is impossible at test facilities, which have combustion heating of flow. Only key criteria, which are significant for the purposes of research, should be simulated exactly.

There was made analysis of different combinations of characteristic parameters. The purpose was to obtain parameter combination, which provides good simulation of engine thrust performances.

Some aspects of the implementation of the measurement system parameters in the conditions of electromagnetic field of high tension

Aleksandrov V Yu, Kozerod A V[@], Zhirnov D B, Kostinsky M A, Moiseev A N and Skomorokhov V S

Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

[@] kozerod@me.com

The generators high-enthalpy flows are used on the ground test facilities to create flow parameters with hypersonic velocities. The generator can include fire, cowper or electric heater depending on necessary conditions. The use of the electric heater with large power leads to the appearance in its vicinity of electromagnetic field of great tension and creates a threat to the influence of electromagnetic interference on system of data acquisition and management. (i) Construction of the 3D model of the test facility with the location of sources of electromagnetic interference and sensing devices. (ii) Creation on the basis of 3D model and pneumatic-hydraulic circuit (PHC) mnemonic scheme of operation of technological systems and test facility components. (iii) The choice of the type of measurement system in accordance with the expected levels of interference. (iv) Correction of placement of transducers and protection of cable paths taking into account sources of interference. (v) The use of fiber-optic communication lines (FOCL) for the implementation of the information highways.

In this work, it is proposed the concrete realization based on VXI and LXI systems for data acquisition. To create PACS and 3D models Autocad, 3ds Max packages were used. For the implementation of the mnemonic scheme special software (SS) Qt-Registrar of Informtest LTD was utilized. The pressure sensors Trafag and STS were used as transducers. The results of experimental studies are presented in this work.

Computational and experimental research of two-phase mixture formation in gasdynamic systems with periodic shock waves

Ananyan M V[1,@], Arefyev K Yu[1,2], Voronetsky A V[2] and Suchkov S A[2]

[1] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] marlen@ciam.ru

High-enthalpy flow generators (HEFG) are widely used in modern power systems, aircraft engines and process installations. HEFG include rocket and jet engines, power plants, high-performance ejectors, airflow combustion heaters, spray coating and cutting machines, etc. From the results of several studies it shows that the creation of highly reliable resonance gas dynamic ignition system (GDIS) is a vital task, because such system will be capable of providing HEFG multiple launch with reasonable boot strap interval. The main advantages of GDIS over other workflow initiation systems are following: the use of the flow kinetic energy for its heating and combustion, expanded operational parameters area, absence of the external energy sources. Within the assigned problem the mathematical models were developed and tested that describe mixing process, evaporation and ignition of the liquid fuel in the unsteady transonic and supersonic oxidizer flow. Calculations allowed to select the geometry of the GDIS duct that provides maximum heat release in a resonant cave stagnant zone (up to 17% of total enthalpy flow through GDIS nozzle). The experimental data were obtained to clarify the features of GDIS physical processes, including fragmentation of liquid droplets in the shock-wave structure and ultrafine two-phase mixture formation. The research was supported by Russian Fundamental Research Fund under research grant number No. 14-08-01118.

Features of radiation-convective heat transfer in the duct with sophisticated shape for multicomponent reacting gas mixture

Frantsuzov M S[1,2]

[1] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

mfrancuzov@yandex.ru

The duct with variable section is considered as an object of research in the present work, where reacting gas mixture under high pressure and different velocities is flowing through this duct. Pressure, temperature and composition were specified on entering of the axisymmetric duct, pressure was specified at the outlet of the duct and duct wall temperature of 800 K was the boundary condition. It was considered the turbulent flow of compressible gas mixture reacted by kinetic mechanisms. Engineering calculation methods also have been used for this duct, where possible. The character and distribution features of convective and radiant heat flux were determined for the range of velocity change. It was defined the maximum portion of radiant heat flux in the total as a function of total flow velocity, static pressure, composition of the combustion products and physical models, which have been used. A comparison of engineering methods based on different generalizations of empirical data. It was found that engineering and computational methods for the determination of the total heat flow give very similar results in some cases.

Particular qualities of radiant heat fluxes calculations for ducts of variable cross-section with supersonic flow

Safonova D B[1,@] and Kukshinov N V[1,2]

[1] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] safonova@ciam.ru

Present work contains the description of methods for calculation of radiant heat flux for high-speed heat-transfer agent. It was carried out calculation research for definition of radiant heat fluxes for ramjet supersonic combustor by several methods. The question of the development of reliable engineering method based on experimental studies and modern physical and mathematical models is considered. The object of research is supersonic combustion chamber through which hydrogen-air fuel mixture flows. Results of numerical simulation of working process in the combustion chamber have been used as an initial data for the calculation of radiant heat fluxes. Numerical simulation was realized in three-dimensional statement, taking into account the turbulence and detailed chemical kinetics. Reynolds averaged Navier–Stokes equations for unsteady turbulent reacting flows were used for solving. For the purpose of describing of hydrogen–air mixture combustion detailed kinetic mechanism of combustion is used. The analysis and comparison of obtained results were carried out. It was defined the difference between radiant heat fluxes magnitudes. This difference can be due to use of various empirical data underlying of every method. Adapted model of radiant heat transfer calculation for supersonic combustion chambers using hydrogen fuel was proposed.

Numerical investigation of one-dimensional approach applicability for hydrogen–air scramjet duct geometry forming

Serpinsky O S[1,2,@] and Kukshinov N V[1,2]

[1] Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] surp9@mail.ru

When developing the scramjets it is significant to choose appropriate geometry of a combustion chamber, which determines conditions of heat release, total pressure losses and, finally, scramjet thrust level. Maximal heat release commonly takes place for the combustion chamber of divergent form.
The object of a present work is to investigate the applicability of one-dimensional approach to the problem of hydrogen–air scramjet duct geometry forming. Using 1D approach three combustion chamber configurations are obtained, of constant static pressure, static temperature and Mach number respectively. For these configurations 2D numerical simulation has been performed. Favre-averaged Navier–Stokes equations are solved and flow is treated as reacting multicomponent mixture with reactions taking place in accordance with multistage kinetic mechanism of hydrogen combustion in air flow. Four different models of chemical kinetics are implemented with subsequent comparison of obtained results.
As the result of research, deviations of respective flow parameters from previously set constant values are obtained for the combustion chamber configurations and thus conclusions concerning applicability of one-dimensional approach for hydrogen-air scramjet duct geometry forming are made.

Different operating regimes of pulse detonation engine simulation

Sidorov R S

Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

sidorov.rodion@gmail.com

The supersonic pulse detonation engines (PDE) can be used as a perspective hypersonic aircrafts propulsion. The engines of this type are expected to have lower heat load and higher thrust-economical characteristics than ramjets at high flight velocities [1]. However the significant difficulties which are connected with both experimental researches and mathematical simulation of physicochemical processes in the PDE occur. In this paper the numerical simulation of different regimes of hydrogen PDE operation is presented. The system of unsteady Reynolds-averaged Navier–Stokes equations for reacting air-hydrogen mixture was resolved numerically. Also the comparison of obtained results with experimental data from detonation burning facility of CIAM [2] was carried out. The dependence of detonation waves passage frequency on excess air ratio in a detonation chamber was chosen as a main comparative criteria.

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On two mechanisms of interaction of high speed cosmic bodies with surface of planets

Barenbaum A A[1,@] **and Shpekin M I**[2]

[1] Oil and Gas Research Institute of the Russian Academy of Sciences, Gubkin Street 3, Moscow 119991, Russia
[2] Kazan Federal University, Kremlyovskaya 18, Kazan, Tatarstan 420008, Russia

[@] azary@mail.ru

When a large cosmic bodies fall on the surface of the planets, may arisen such big pressures, that the strength and plastic properties of medium and the friction forces can be ignored compared to the inertial forces. In these circumstances, the impact process can occur by two different mechanisms [1], which we can name the approximations of "elastic" and "inelastic" shock. In the case of "elastic" shock, the main part of the kinetic energy and impulse of the cosmic body is spent on the crater formation [2]. When shock is "inelastic", the energy and impulse of cosmic body are passed to narrowly-focused shock wave, which penetrates deep into the lithosphere of the planet, expending its energy on evaporation, melting and heating of lithosphere rocks [3]. Such a model well explains the origin on Earth and Venus geological structures formed by falls of high-speed galactic comets [4]. This question is discussed on basis of the analysis of high resolution images of some craters on Moon, where we have detected evidences [5] of action the "elastic" and "inelastic" mechanisms.

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3. Power Interaction with Matter

Cavitation and spallation of a liquid layer in gold irradiated by femtosecond laser pulse

Ashitkov S I[1,@], Komarov P S[1], Zhakhovsky V V[2], Inogamov N A[3] and Agranat M B[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] All-Russia Research Institute of Automatics named after Dukhov, Luganskaya 9, Moscow 115304, Russia
[3] Landau Institute for Theoretical Physics of the Russian Academy of Scienses, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia

[@] ashitkov11@yandex.ru

We report on the ablation phenomena in gold sample irradiated by femtosecond laser pulses of moderate intensity. The dynamics of expansion of a heated surface layer was investigated in a picosecond range using ultrafast chirped interferometry. Also the morphology of ablation craters and the value of ablation threshold (for absorbed fluence) were measured. The experimental data are compared with the simulation of a mass flows obtained by two-temperature hydrodynamics and molecular dynamics methods. Simulation shows evolution of a thin surface layer pressurized after electron–ion thermalization, which leads to melting, cavitation and spallation of a part of surface liquid layer. The experimental and simulation results on a fracture, surface morphology and strength of liquid gold at a strain rate $\sim 10^9$ s^{-1} are discussed.This work was supported by the Russian Science Foundation, grant number 14-50-00124.

Ablation of iron irradiated by femtosecond laser pulses

Struleva E V[@], Ashitkov S I, Komarov P S, Khishchenko K V and Agranat M B

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] struleva.evgenia@yandex.ru

Our understanding of femtosecond laser interactions with metals based on the two temperature model [1]. Since the heat capacity of the electrons is much smaller than that of the lattice, an ultrashort laser pulse with a duration less than the heating time of the lattice can heat electrons in a metal to a very high temperature while leaving the lattice relatively cool. Ultrafast heating the thin surface layer of metal target gives rise to powerful tensile stresses and ablation nanolayer of material [2]. In the current work ablation thresholds and morphology of the surface have been measured for iron by means of femtosecond interferometric microscopy [1]. Using an interferometric continuous monitoring technique, we have investigated the motion of the surface of an iron target in the case of femtosecond laser ablation at picosecond time delays relative to the instant of laser exposure. The experimentally determined value of the tensile stresses that lead to the separation of layer of material for different fluence. Measurements of the temporal target dispersion dynamics and the morphology of the ablation crater have demonstrated thermomechanical nature of the fracture of the condensed phase because of the cavitation-driven formation and growth of vapour phase nuclei upon melt expansion, followed by the formation of surface nanostructures upon melt solidification. This work was supported by the Russian Science Foundation grant No. 14-50-00124.

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Reflectance of thin silver film on the glass substrate at the interaction with femtosecond laser pulses

Petrov Yu V, Khokhlov V A and Inogamov N A[@]

Landau Institute for Theoretical Physics of the Russian Academy of Scienses, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia

[@] nailinogamov@gmail.com

The optical response of thin silver film (60 nm thickness) coated on a glass prism (Kretschmann configuration) and heated by the femtosecond laser pulse of small intensity is investigated by the computational modeling. We have calculated the reflectance of p-polarized probe laser beam when it is incident onto the metal film from the glass side. Reflectance is calculated at incidence angles close to the surface plasmon resonance angle. We have considered first 100 ps after the action of femtosecond laser pulse onto the film surface. Changes in thermodynamic state and hydrodynamic motion of film matter are described by the system of hydrodynamic equations taking into account different temperatures of electrons and ions (two temperature state) and consequently two temperature thermodynamics and kinetics at such early times. These changes define the changes in electron-ion and electron-electron collision frequencies. Calculated in dependence on the density and electron and ion temperatures, these frequencies allow us to find the intraband (Drude) part of dielectric permittivity. Together with the interband contribution it gives possibility to calculate reflectance in dependence on the state of metal surface. It is shown a great importance of electron-electron interactions in the temporal behavior of reflectance at early times of laser-film interaction. Authors are grateful for support from RFBR 16-02-00864 A.

Metal film on substrate: Dynamics under action of ultra-short laser pulse

Khokhlov V A[1,@], Anisimov S I[1], Inogamov N A[1], Zhakhovsky V V[2,1] and Khishchenko K V[3]

[1] Landau Institute for Theoretical Physics of the Russian Academy of Scienses, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia
[2] All-Russia Research Institute of Automatics named after Dukhov, Sushchevskaya 22, Moscow 127055, Russia
[3] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] v_a_kh@mail.ru

Many laser experiments are carried on the targets composed from a film mounted on a dielectric or semiconductor substrate. Therefore this problem is significant. In the literature the bulk targets (BT) or freestanding films (FSF) are considered mainly. These two cases differ qualitatively from the film/substrate (F/S) case considered here. In the BT the phenomenon of the rear-side spallation is absent; while there are no dynamic influence from the substrate in the FSF (vacuum from the both sides). The parameter d_f/d_T and absorbed fluence $F_{\rm abs}$ parameterize dynamics of ablation (irradiated side) and spallation (rear-side) of the FSF (Demaske et al., PRB **82**, 064113 (2010)), here d_f, d_T are thicknesses of a film and a heat affected layer. In our Elbrus last year's paper Khokhlov et al., J. Phys. Conf. Ser. **653**, 012003 (2015) the oscillations and the separation of a thin ($d_f < d_T$) film *as whole* from substrate have been studied. Here we consider, firstly, transition from the regime of separation as whole to the regime of the internal breaking of a film and, secondly, the influence of the parameter d_f/d_T on motion. Two breakings appear (if $F > F_{\rm spall} > F_{\rm abl}$) if a film is thick $d_f > d_T$, here $F_{\rm spall}, F_{\rm abl}$ are the spallation and ablation thresholds, resp. The first breaking is ablation in the rarefaction wave on the irradiated side, while the second breaking is a spallation near the F/S contact. In the thin films these two breakings merge together, see Demaske et al. (2010) cited above.

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Heating of an aluminum target by femtosecond laser pulse: Two-dimensional simulations

Shepelev V V[1,2] **and Inogamov N A**[2,@]

[1] Institute for Computer-Aided Design of the Russian Academy of Sciences, Vtoraya Brestskaya 19/18, Moscow 123056, Russia
[2] Landau Institute for Theoretical Physics of the Russian Academy of Scienses, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia

[@] nailinogamov@gmail.com

We consider illumination of 200 nm thick Al film by a single femtosecond laser pulse in two-dimensional (2D) geometry. Energy $F_{\rm abs}$ per unit area absorbed in a skin layer is harmonically modulated along a surface $F_{\rm abs} = F_0 + \Delta F \cos ky$, where the axis y is directed tangentially along a surface, ΔF is an amplitude of modulation. Full two-temperature (2T) physics (including a 2T heat conduction coefficient $\kappa(T_e, T_i)$ and an electron-ion coupling parameter α together with a 2T equation of state and melting/solidification) is used in simulations. Two coupled thermal equations are solved. They are equations for energies of the electron and ion subsystems taken from the pioneer work by Anisimov *et al* 1974 *JETP* but now in 2D geometry. 2D 2T thermal equations take into account transverse electron thermal flux $q_\perp$ dumping the non-homogeneity of the distribution of $F_{\rm abs}$ along a surface. Of course, efficiency of dumping depends on the ratio of wavelength $\lambda = 2\pi/k$ and thickness of a heat affected surface layer d_T. At $\lambda/d_T \gg 1$, the hotter and colder parts of a surface are too far from each other to be influenced by a weak in this case transverse conductance. In the opposite limit, the inhomogeneous case does not differ from the homogeneous one (fast dumping). The paper presents quantitative studies of this problem. The problem helps us to understand, how and at what spatial scales the surface perturbations will survive. The relative roles of the flux $q_\perp$ at the supersonic 2T stage and at the subsonic one-temperature (1T) stage are estimated. Authors acknowledge the support from Russian Science Foundation (grant No. 14-19-01599).

A comparison of atomistic and continual simulation of ablation dynamics under femtosecond double-pulse laser irradiation of metals

Fokin V B[@], Povarnitsyn M E and Levashov P R

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] Vladimir.Fokin@phystech.edu

We perform a numerical simulation of double femtosecond laser pulse action on metals using two methods: (i) a two-temperature one-velocity hydrodynamic model (HD) [1] and (ii) a modified combined model, which is based on the molecular-dynamics approach for ions and on the heat conduction equation solution for electrons (TTM-MD) [2]. These models both take into account electron-phonon coupling, laser energy absorption, and electronic heat conductivity, so they are able to describe the second laser pulse absorption correctly. The TTM-MD accurately reproduces nonequilibrium phase transitions and surface effects on nanoscale. The HD demonstrates good qualitative agreement with the TTM-MD in the dynamics of phase explosion and spallation. In this work we have suggested two mechanisms of suppression of ablation responsible for the monotonic decrease of the ablation crater depth when the delay between pulses increases (this effect was registered experimentally in [3]). The results of both simulations (HD & TTM-MD) of the double-pulse ablation obtained for different delays from 1 to 100 ps correlate with the experimental findings. Other advantages and disadvantages of both approaches are examined and discussed.

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Molecular dynamics simulation of cavities in aluminum melt at tension

Avdeeva A V

Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia

awdeewaanya@yandex.ru

High-energy irradiation of the metal causes the melting of the material and the increasing of the pressure in the areas of greatest heating. The resulting melt begins to expand under the pressure, passes into the metastable state before the start of the process of destruction due to the formation and growth of cavities. It is necessary to study the dynamics of cavities for the description of the process of destruction of this system.

A character of variation of the radius of existing cavity that is predicted by the continuum model [1] is verified in this work. Parameters of this model are fitted to the best correspondence with the molecular dynamics (MD) simulations for the strain rate 1/ns. All calculations are performed for Al melts within a wide range of initial radius of the cavities (from 3 lattice constants to 15 lattice constants) at the temperatures 1000, 1500, 2000 and 2500 K. The molecular dynamics simulator LAMMPS [2] with the interatomic potential [3] is used for MD simulations.

The work was supported by the grant from the Russian Science Foundation (Project No. 14-11-00538).

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Dynamics of laser ablation at the early stage during and after femtosecond pulse

Ilnitskiy D K[1], Khokhlov V A[2], Zhakhovsky V V[1] and Inogamov N A[2,1,@]

[1] All-Russia Research Institute of Automatics named after Dukhov, Luganskaya 9, Moscow 115304, Russia
[2] Landau Institute for Theoretical Physics of the Russian Academy of Scienses, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia

[@] nailinogamov@gmail.com

Two-temperature hydrodynamics codes are used to explore phenomena at the very early stage of laser action covering duration of a laser pulse and few first picosecond. Work is supported by the Russian Science Foundation, grant No. 14-19-01599.

Blistering of film from substrate after action of femtosecond laser pulse

Zhakhovsky V V[1] and Inogamov N A[2,1,@]

[1] All-Russia Research Institute of Automatics named after Dukhov, Luganskaya 9, Moscow 115304, Russia
[2] Landau Institute for Theoretical Physics of the Russian Academy of Scienses, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia

[@] nailinogamov@gmail.com

To explain experimental results concerning film blistering—this is the goal of the report. Work is supported by the Russian Science Foundation, grant No. 14-19-01599.

Transport properties of copper with excited electron subsystem

Petrov Yu V[1,2], Migdal K P[3,@], Knyazev D V[2,4,5], Inogamov N A[1,3] and Levashov P R[4,6]

[1] Landau Institute for Theoretical Physics of the Russian Academy of Scienses, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
[3] All-Russia Research Institute of Automatics named after Dukhov, Sushchevskaya 22, Moscow 127055, Russia
[4] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[5] State Scientific Center of the Russian Federation "Institute for Theoretical and Experimental Physics", National Research Center "Kurchatov Institute", Bolshaya Cheremushkinskaya 25, Moscow 117218, Russia
[6] Tomsk State University, Lenina Avenue 36, Tomsk 634050, Russia

[@] migdal@vniia.ru

We have investigated transport properties of an electron subsystem of copper heated by a femtosecond laser pulse. These properties change greatly in comparison with the room temperature solid metal. The electron temperature and pressure profiles significantly depend on these properties in bulk laser targets according to the two-temperature (2T) model. These profiles at the 2T stage are responsible for shock and rarefaction waves formation. We have developed the analytical model of electroconductivity and heat conductivity of copper which takes into account changes of density, electron and ion temperatures. The model is based on the solution of the Boltzmann equation in the relaxation time approximation for consideration of electron collisions. Also we have carried out the first-principles calculations using the Kubo–Greenwood theory, methods of psedopotential and linear augmented plane waves which are necessary to evaluate electron wavefunctions. We have provided the check of convergence of all parameters of our first-principles calculations. The results of our analytical model for electro- and heat conductivities are in good agreement with the data obtained using the linearized augmented plane wave (LAPW) method. PYV, MKP, and INA acknowledge RFFI for support (grant 16-02-00864).

Laser-induced Coulomb explosion of aluminium nanoclusters: Wave packet molecular dynamics

Orekhov N D[@] and Stegailov V V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] stegailov@gmail.com

The interaction of ultrashort laser pulses with nanoclusters has recently become a subject of interest due to efficient laser radiation absorption with an energy capture per atom much higher than for bulk material. In combination with small cluster sizes and low levels of energy losses, it allows to product nanoplasmas and high-energy particles. Here we apply eFF potential to calculate the properties of electronically exited Al nanoclusters. eFF is based on a simplified solution to the time-dependent Schrrodinger equation with a single approximate potential between nuclei and electrons. It provides the combination of molecular dynamics with the methods of wave packet dynamics representing electrons as floating Gaussian wave packets and nuclei as classical particles.

We examine the mechanisms of Al nanoclusters ionization and explosion under different intensities and durations of laser pulse. For system sizes up to several thousand atoms, thresholds for cluster explosion are calculated. For laser intensities below the threshold, rate of electron-ion temperature equilibration in forming nanoplasma and its dependence on laser pulse duration is discussed.

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A wide-range model for simulation of laser-induced dynamics of aluminum plasma

Povarnitsyn M E[@] and Andreev N E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] povar@ihed.ras.ru

We use a wide-range model [1] of optical and transport properties for simulation of laser-induced dynamics of aluminum plasma. The model describes laser energy absorption, electron thermal conductivity, two-temperature effects of electron-ion collisions as well as hydrodynamic motion of matter. The model successfully describes pump-probe experiments [2], experiments on self-reflectivity in wide range of intensities [3, 4], and angular dependence of reflectivity coefficient for S- and P-polarized pulses [5]. Thus, we can reliably predict the main parameters of aluminum plasma such as temperature, density, velocity, mean charge of ions for optimization of planned experiments.

The work is supported by the Russian Science Foundation grant No. 14-50-00124.

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Hot electrons generation in the laser–plasma interaction at relativistic intensities

Andreev N E[@], Pugachev L P and Povarnitsyn M E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] andreev@ras.ru

The generation of hot electrons in the interaction of a subpicosecond relativistic-intense laser pulse with solid targets is analyzed for the parameters of petawatt class laser systems. We study the preplasma formation on the surface of solid Al target produced by the laser prepulses with different time structure depending on the laser angle of incidence. The preplasma dynamics was analyzed using a wide-range two-temperature hydrodynamic model for different contrast ratios of the nanosecond pedestal.

The electron acceleration by the main p-polarized laser pulse was modeled in three dimensional particle-in-cell (3D PIC) simulations. The effective hot electron temperatures are determined for normal and grazing laser pulse incidence and compared with known scaling of characteristic energies of laser accelerated electrons.

Optimization of electron acceleration under the action of petawatt-class laser pulses onto foam targets

Pugachev L P[@], Andreev N E and Levashov P R

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] puleon@mail.ru

Optimization study for future experiments on interaction of the PHELIX petawatt laser pulses with foam targets was done by 3D PIC simulations. Densities in the range $0.5n_c$–n_c and thicknesses in the range 100–500 μm of the targets were considered corresponding to those which are currently available. Accelerated electrons are obtained with the temperature 8.5 MeV and the maximal energy 100 MeV. The charge contained in electrons with energies higher than 30 MeV is about 30 nC. It is shown that heating of electrons mainly occurs under the action of the ponderomotive force of a laser pulse whose amplitude increases up to three times because of self-focusing. Accelerated electrons gain additional energy directly from the high-frequency laser field at the betatron resonance in the emerging plasma density channels. For thicker targets higher number of electrons with higher energies is obtained. The narrowing of the angular distribution of electrons for thicker targets is explained by acceleration in multiple narrow filaments.

Trapping and acceleration of the electron bunch in a wake wave

Kuznetsov S V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

shenau@rambler.ru

The process of electron trapping by a wake wave excited by a laser pulse in a plasma channel in the case where the electron bunches are injected into the vicinity of the maximum of the wakefield potential at a velocity lower than the wave phase velocity is considered [1–3]. The mechanism for the formation of a compact electron bunch in the trapping region when only the electrons of the injected bunch that are trapped in the focusing phase mainly undergo the subsequent acceleration in the wakefield is analyzed. The influence of the spatial dimensions of the injected bunch and its energy spread on the length of the trapped electron bunch and the fraction of trapped electrons is studied analytically and numerically. For electron bunches with different ratios of their spatial dimensions to the characteristic dimensions of the wake wave, the influence of the injection energy on the parameters of the high-energy electron bunch trapped and accelerated in the wakefield is studied.

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Laser wakefield acceleration of polarized electron beams

Pugacheva D V[1,2,@], Andreev N E[1,2] and Cros B[3]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
[3] Laboratoire de Physique des Gaz et des Plasmas, Universite Paris Sud 11, Rue Henri Becquerel 210, Orsay 91405, France

[@] sedyakina.d@gmail.com

The acceleration of highly polarized electron beams are widely used in state-of-the-art high-energy physics experiments [1]. In this work a model for investigation of relativistic electrons spin precession in the laser-plasma accelerator depending on the initial energy of electrons and its injection phase was developed and tested. To obtain the evolution of the trajectory and momentum of the electron for modeling its acceleration the wakefield structure was determined. The spin precession of this electron was described by Thomas–Bargman–Michel–Telegdi (T-BMT) equations [2]. Optimal parameters providing minimum depolarization of the electron, when it is accelerated in the wake wave generated by a laser pulse, were found. With these parameters the evolution of the electron beam polarization was investigated and the influence of beam emittance on its depolarization during the acceleration was examined.

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On the control of geometric factors for high quality accelerated electron bunches in guiding structures

Veysman M E[@], Andreev N E and Kuznetsov S V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] bme@ihed.ras.ru

Guiding structures (evacuated capillary waveguides with inner radiuses comparable to laser pulses spot radiuses or plasma channels formated in gas-filled capillaries with much wider inner radiuses) are known to be effective tools for laser pulses propagation over many Releigh length and laser wakefield electron acceleration [1–9]. We had studied the characteristics of electron bunches accelerated in wakefields of laser pulses, propagating in different guiding structures, in the case of different non-symmetric conditions of laser pulses focusing into an entry of the guiding structure. This study is essential for the modern concept of creation of table-top laser wakefield accelerators, as long as it is relevant to real experimental situation. The maximum adoptable inaccuracies of laser pulse focusing into a channel, in connection of the task of obtaining qualitative accelerated electron bunches (with high energy, low energy spread) are discussed.

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Experimental verification the ablation pressure dependence from the intensity of the laser radiation with duration of 70 ps

Stuchebryukhov I A[1,@], Krasyuk I K[1], Semenov A Yu[1] and Khishchenko K V[2]

[1] Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova 38, Moscow 119991, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] st777@kapella.gpi.ru

The experimental verification of the relation of ablation pressure on the front surface of the target with the intensity of the laser used in the papers [1, 2] was done. The experiments were performed on a terawatt laser system "Kamerton-T" (GPI). As a result the arriving time of shock-wave front on the free (rear) of the target surface of copper and aluminum was measured. For the experiments, an optical system was used in which the probe laser beam directs at the back side of the target in shock-wave zone. The output of the shock waves on the surface was determined by the change in the character of the probe laser radiation reflection. The experimental values of the laser pulse energy, duration and size of the ablation spot on the front surface of the target was used for calculation the laser intensity on the target. And then using the test scaling formula the amplitude of ablation pressure on the front surface of the target was determinate. This value is compared with calculated amplitude of the pressure, at which the shock wave arriving coincides with the value obtained experimentally. As a result, it found that the error in determining the amplitude of the ablation pressure when using the scaling does not exceed 9%.

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Non-ideal plasmas created in the short pulse laser interaction with mass-limited and nanostructured targets

Rosmej O N[1,@], Neumayer P[1], Khaghani D[1], Schönlein A[1] and Pikuz S A[2]

[1] GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, Darmstadt 64291, Germany

[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] o.rosmej@gsi.de

Petawatt PHELIX-laser system at the Gesellschaft für Schwerionenforschung GSI-Darmstadt is an important instrument for creation and investigation of a wide range plasma states, from ideal plasmas of intermediate densities and few keV temperatures up to so called warm dense matter. The variety of experiments on the generation of non-ideal plasmas by isochoric heating of mass limited and nanostructured solid targets by the laser accelerated electrons have been carried out. The achieved plasma parameters, analyzed by means of highly resolved x-ray spectroscopy of the target K-shell radiation, demonstrate a high level of the plasma non-ideality and up to Gbar dynamical plasma pressure.

Theoretical and experimental studies of the radiative properties of plasma and their applications to temperature diagnostics for low Z and high Z element plasmas

Orlov N Yu[1,@], Denisov O B[1], Vergunova G A[2] and Rosmej O N[3]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia
[3] GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, Darmstadt 64291, Germany

[@] nyuorlov@mail.ru

Important features of the theoretical model, known as the ion model (IM) of plasma, which is used for quantum mechanical calculations of radiative opacity, are discussed. Reliability of IM results was tested with experiment, where measurements of x-pinch radiation energy yield for two exploding wire materials, NiCr and Alloy 188 were made. Theoretical estimations of radiative efficiency were compared with experimental results, and IM calculations agree well with the experimental data. Subsequently, the theoretical approach was used for temperature diagnostics of CHO plasma target in combined laser—heavy ion beam experiments. As it was found, the theoretical approach can be used for temperature diagnostics of high Z element plasmas in Z-pinch. Calculations of the spectral brightness were made for Mo plasma radiation at the temperatures 1 and 1.2 keV and the densities 1 and 2 g/cc.

Laser energy conversion efficiency to hot electrons in the interaction with metal targets

Kostenko O F[1,@], Andreev N E[1], Rosmej O N[2] and Schönlein A[3]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, Darmstadt 64291, Germany
[3] Goethe University Frankfurt am Main, Grüneburgplatz 1, Frankfurt am Main 60323, Germany

[@] olegkost@ihed.ras.ru

Experiments at the GSI with high intensity laser system PHELIX have been aimed at the investigation of generation of the 22.1 keV Ag K_α radiation for radiographic applications. In order to exclude a process of the electron refluxing from the analysis of the Ag K_α generation, the bulk Ag target was used. Application of silver foils, attached onto the low-Z substrates, led to strong reduction of bremsstrahlung radiation level, what was important for increasing of the accuracy of the absolute K_α measurements. The laser intensity was varied in the range between 10^{18} and 2×10^{19} W/cm^2.
We have applied the model of characteristic x-rays generation by laser produced relativistic electrons propagating in a metal target to reveal an intensity dependence of the conversion efficiency of laser energy into hot electrons using measurements of the absolute K_α yield per unit laser energy. We take into account the intensity dependence of the effective hot electron temperature using the ponderomotive scaling.
The intensity dependences of the K_α yield, calculated using determined conversion efficiency with the assumption of suppression of hot electron refluxing, describe well features revealed in the experiment. The calculations with refluxing electrons confirm the assumption about suppression of hot electron refluxing in the foils deposited on the bulk substrates, both conducting and nonconducting.

Parameters of supersonic astrophysically-relevant plasma jets collimating via poloidal magnetic field measured by x-ray spectroscopy method

Filippov E D[@], Pikuz S A, Skobelev I Yu and Ryazantsev S N

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] nopers@bk.ru

Application of magnetic field allows to investigate large aspect ratio jets which are related with the several astrophysical cases [1]. In the experiment with 0.6 ns, 40 J laser pulses focused to 700 μm focal spot at solid CF_2 target in presence of 20 T poloidal magnetic field the parameters of the plasma jet were studied by means of spatially resolved x-ray spectroscopy with spatial resolution along the jet propagation. Using the method [2] which considers the relative intensities of spectral lines emitted by F He-like ions, the electron temperature T_e and density N_e profiles of the plasma are obtained. It is shown that N_e decreases monotonically in the case without B-field, but demonstrates an extended density profile up to 10 mm when 20 T magnetic field is applied. N_e values are consistent with that observed via interferometry diagnostics, thus providing the confidence in our x-ray spectroscopy analysis techniques. While at the laser irradiated target surface T_e peaks at 250–280 eV, at 3 mm distance it cools down to $\sim$ 20 eV. Then, due to the impact of B field providing the collimation of the jet, T_e and N_e are measured to keep at almost constant values along many mm's along the jet.

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Radiation dominant kinetic regime in the plasma created by the intense ultrashort laser pulse

Pokrovskiy G V[1,2,@], Pikuz S A[1,3] and Alkhimova M A[1,3]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
[3] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

[@] george.pokrovskiy@gmail.com

In the series of experiments conducted in April of 2015 at the PEARL facility in the Institute of Applied Physics (Nizhniy Novgorod, Russia), in the year 2014 at the J-KAREN facility (Kansai, Japan) and in the year of 2013 at the Vulcan facility (Rutherford, United Kingdom) a new exotic state of matter was obtained.The focusing spectrometer registered spectral lines which belong to the KK- and KL-hollow ions.
For the description of x-ray propagation the concept of the radiation dominant kinetic regime (RDKR) was involved which previously had been suggested for the description of kinetic processes in the plasma. According to the RDKR model all the plasma area is divided into 3 Zones with different parameters such as electron temperature and density. The laser beam is focused into the central Zone and thus creates electrons which reflect many times from the surfaces of the target. The electrons produce x-ray photons going to the periphery of the plasma with solid density. According to estimates, the central Zone and the peripheral Zone have electron temperatures of 60 eV and 10 eV respectively. It is the periphery of the plasma area where the hollow ions are produced.
One can state that diffusion of the x-ray radiation from the center to the periphery takes place. This is the RDKR within which kinetic processes are defined by the x-ray radiation propagating in the plasma.

Determination on spectral reflectivity of spherically bent mica crystals applied for diagnostics on relativistic laser plasmas

Alkhimova M A[1,2,@], Pikuz S A[1,2], Faenov A Ya[1,3] and Skobelev I Yu[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[3] Institute for Academic Initiatives, Osaka University, Yamadaoka 1-1, Suita, Osaka 565-0871, Japan

[@] MAAlkhimova@mephi.ru

Mica crystals are widely applied in x-ray spectroscopy diagnostics since their ability to effectively reflect the radiation in different orders covering a wide range of photon energy, including sub-keV range hardly accessible with other crystals. Particularly, spherically bent mica crystals are commonly used in high energy density plasma imaging spectrometry diagnostics. However, the detailed reflectivity properties of bent mica crystals are not known well. Here we propose and verify the way to calibrate mica crystal spectral reflectivity in the experiment with relativistic laser plasma. The approach is based on the comparison of dense laser plasma x-ray spectra measured by focusing spectrometers with spatial resolution (FSSR) equipped, with examined mica and pre-calibrated alpha-quartz bent crystals. As a result, the normalized reflectivity of spherically bent mica crystal operated in 2-nd order of reflection was experimentally evaluated for the first time versus wavelength in the range of 6.7–8.7 Å. The obtained spectral calibration curve for bent mica crystal demonstrates remarkable difference to that one calculated for flat mica crystal and given in Henke tables [1], and has to be applied further for a correct interpretation of the measured x-ray spectra.

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Spatial configuration of fast ion source in femtosecond laser plasma of cluster targets

Makarov S S[1,@], Pikuz S A[2], Skobelev I Yu[2], Faenov A Ya[2], Pikuz T A[2] and Varzar S M[1]

[1] Faculty of Physics of the Lomonosov Moscow State University, Leninskiye Gory 1 Bldg 2, Moscow 119991, Russia

[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] seomakarov28@gmail.com

The method of ion radiography is widely used for monitoring in micro- and nanotechnology production as well as for diagnostics of ultrafast processes in high energy density physics research. Femtosecond laser-produced plasma is one of the most promising compact sources of fast ion beams. In this context, gas cluster targets possess a number of practical advantages. For radiography applications the uniformity of the probe ion beam in a wide solid angle is important. Respectively, for the further development of ion radiography techniques it is necessary to determine the spatial structure of the ion source generated in femtosecond laser plasma. This work is aimed to study the spatial configuration of the ion source generated by 36 fs laser pulses of 160 mJ energy fosed in CO_2 cluster target. To register an image of the ion source two pin-holes coupled with CR-39 track detectors are used. It was shown the source configuration depends on the laser focusing position in the cluster cloud. For the first time it was obtained that the image of the plasma region with a maximum fast ion yield is spatially separated from that one with peaked yield of x-rays (considered to be the best focus of the laser). The assumption is done and now being verified that such image separation is caused by the influence of the magnetic field occurring near the plasma channel in cluster cloud and affecting the ion flux from the source to the detector. For consideration the magnetic field configuration was taken from PIC laser plasma modeling. Magnetic field strength and spatial scale required to describe the observed configuration of the ion source image are estimated.

Diagnostics of recombining laser plasma parameters based on He-like ion resonance lines intensity ratios

Ryazantsev S N[1,@], Skobelev I Yu[1], Faenov A Ya[1], Pikuz T A[1], Grum-Grzhimailo A N[2] and Pikuz S A[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Skobeltsyn Institute for Nuclear Physics of the Lomonosov Moscow State University, Leninskiye Gory 1, Moscow 119899, Russia

[@] sergryaz@mail.ru

Laser produced jets are fully scalable to YSOs because of the plasma evolution equations invariance under some transformations [1]. While the plasma created by powerful laser expands from the target surface it becomes overcooled, i.e. recombining one. So to improve diagnostic methods applicable for such plasma is rather important problem in laboratory astrophysics.

Intensity ratios of x-ray resonance lines radiated by multicharged ions can be used for plasma diagnostics. Mentioned ratios can be calculated in terms of quasi steady-state approximation for the wide range of densities and temperatures. Comparing the ratios obtained from a real plasma spectrum with calculated values it becomes possible to evaluate plasma parameters.

The method was applied to successfully interpret the spectra of F VIII ions emitted by laser plasma jet created from CF_2 solid target irradiated by ns 10–60 J laser pulses [2]. It was shown intensity ratios are sensitive to the density in the range of 10^{16}–10^{20} cm^{-3} while the temperature ranges from 10 to 100 eV for ions.

Method allowed to determine plasma parameters rather far from the target surface. Sensitivity of the method was proved to be enough to distinguish the difference between parameters of plasma jets for various geometries in the experiment.

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On the reflection properties of focusing x-ray crystals

Baronova E O[@], Lomov A A and Subbotin I A

Institute of Nuclear Synthesis of the Russian Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia

[@] baronova04@mail.ru

Concave x-ray crystals are key elements of Johann focusing spectrometers widely used in plasma diagnostics. Resolution of such spectrometers depends on the diffraction properties of bent crystals. The shape of rocking curve was studied within Takagi–Taupin equations. It was shown that rocking curve becomes wider for smaller crystal radii. The results of calculations are supported by experimental one: experimental study of list of concave crystals are also presented. Finally the code is designed to simulate the shape of rocking curves of bent crystals. Such code is aimed to predict diffraction properties of concave crystal samples and also to estimate the resolution of focusing x-ray spectrometers in case of point-like sources, situated at the distance from Rowland circle.

X-ray photoelectron spectroscopy in research of sodium chloride after laser effects

Savintsev A P[@], Gavasheli Yu O, Kalazhokov Z Kh and Kalazhokov Kh Kh

Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia

[@] pnr@kbsu.ru

In a unique setup "Laser Femtosecond Complex" of the Joint Institute for High Temperatures Research RAS [1], carried out is the impact on the surface of an ionic crystal laser radiation with intensity more than 50 TW/cm^2 [2]. Femtosecond laser pulses at a wavelength of 800 nm leads to optical damages (craters) on the sample surface. To analyze the effects of exposure to the laser effects used x-ray photoelectron spectrometer "Termo Scientific K-Alpha". Samples were loaded into the chamber of the spectrometer, where the vacuum was of the order of 10^{-9} mbar. In the case study of the surface elemental composition [3], the concentration of the sample components was determined with an accuracy of $\pm 0.3\%$. The energy of the electrons [4] at the site was up to ± 0.2 eV. Explore the surface of the crater and other surface, before and after cleaning the ion bombardment with argon ions of the crystal. Comparative analysis of XPS spectra showed that in the case of sodium chloride, high-intensity laser radiation affects the energy of the electrons in the atoms on the surface and the composition of the surface of an ionic crystal. This work was supported in the framework of the base part of the Russian Ministry goszadaniya KBSU in the years 2014–2016 (project 2014/54-2228).

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Analysis of ablation pressure created laser pulses

Gavasheli Yu O, Savintsev A P[@] and Gavasheli D Sh

Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia

[@] pnr@kbsu.ru

Earlier we have to analyze very rapid destruction of an ionic crystal surface data were used, which relate to the ablative destruction portion [1, 2]. Ablation is characterized by certain regularities, and ablative values of pressures can be used to investigate the damage threshold dependence of the pulse duration, for example, such a crystal as sodium chloride [2]. To calculate the ablation pressure p_a used two formula [3, 4]: (1) $p_a(\text{kbar}) = 4.8 \times 10^{-4}(I, \text{W/cm}^2)^{1/2}$, and (2) $p_a(\text{Mbar}) = 12(I/10^{14}, \text{W/cm}^2)^{2/3}(\lambda, \mu\text{m})^{-2/3}$, where I—intensity of the laser pulse, and λ—the wavelength of the laser radiation. The calculations were performed for two wavelengths $\lambda_1 = 1240$ nm, $\lambda_2 = 800$ nm and a value $I = 50$ TW/cm^2 [5, 6]. Calculation by formula (1) gives $p_a = 3.4$ Mbar, and the formula (2)—$p_{a1} = 6.6$ Mbar and $p_{a2} = 8.8$ Mbar. The values obtained are of great interest, because at such pressures on the surface of the sodium chloride may have a transition dielectric–metal [5, 7].

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Ultrafast destruction of the quartz optical fibers under laser radiation

Efremov V P[@], Frolov A A and Fortov V E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] dr.efremov@gmail.com

This work is directed to the study of destruction features of quartz optical fiber under intense laser radiation. We have used experimental quartz optical fibers manufactured in Fiber Optics Research Center of the Russian Academy of Sciences and industrial quartz optical fibers for communication.

There are two modes of propagated damages caused by laser radiation in silica-based optical fibers. At detonation-like mode the plasma front is two orders of magnitude greater than for a fiber fuse effect (combustion mode). This mode is new object of laser destruction of silica-based optical fibers. Optical fiber and enough long laser pulse let us obtain laser damage propagated more than hundred fiber core diameters during pulse. The optical fibers application provides the some advantages. It allows supply the same form of energy deposition in the every cross section of optical fiber. Tested regime demonstrates near constant velocities during 200 ns in the range of laser intensity 2–4.5 GW/cm^2. Plasma propagation produced irreversible damages in the optical fiber. Saved fragments were investigated by a scanning electron microscope. Melted and crushability zones have been visualized and measured. Dynamic recordings of destruction process were compared with photos of the saved fragments. It has been received that destruction of a core and cover of quartz optical fibers has multilevel character from the micron size to nanodestructions. This work has been done due to support of Presidium RAS program.

The glass nanocomposites optical strength laser ablation studies

Shemanin V G[@] and Mkrtychev O V

Novorossiysk Polytechnic Institute of the Kuban State Technical University, Karl Marx 20, Novorossiysk 353900, Russia

[@] vshemanin@mail.ru

The theoretical and experimental studies results of the glass nanocomposites' optical strength in [3] shows the influence of physical factors on the optical strength. The optical strength prediction is based on Weibull–Gnedenko's statistical distribution with the stochastic properties of the laser ablation breakdown at the nanocomposite surface [2]. The conclusions, related to The single laser irradiation result at the sample [3] can be applied to predict sample optical strength at the multiple laser pulses irradiation. According to the results the time when the sample reliability R is achieved $1/e$ at the irradiation with the pulses energy density F and laser pulse repetition rate f can be calculated by the formula

$$t(R, F, m) = \frac{1}{f} \frac{F_{0.5}^m}{F^m} \frac{\ln(1/R)}{\ln 2}.$$

The parameters $F_{0.5}$ and m are determined from the experimental results [3]. For the studied samples have been found that the irradiation time duration when the optical strength decays up to $R = 1/e$ varies in the range from 1.6 to 8270 s with the laser pulse duration of 20 ns and the energy in the range of $15 \ldots 30$ mkJ. Therefore the treatment algorithm of the nano film reliability with the experimental results in the small measurements party [3] on the basis of Weibull–Gnedenko statistical distribution was developed and it allows to predict the glass nanocomposites optical strength dynamics.

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The optical strengths of the glass composite with sol-gel nanofilms

Atkarskaya A B, Zakalova E Yu, Kaunov V S, Nartsev V M, Chartiy P V and Shemanin V G[@]

Novorossiysk Polytechnic Institute of the Kuban State Technical University, Karl Marx 20, Novorossiysk 353900, Russia

[@] vshemanin@mail.ru

The optical and mechanical strength values dependence of the glass composites with the nanofilms drawn from the sols, the films thickness, the dispersed phase particles packing density in the sol layer and these particles diameter have been studied in this work. The optical strength was determined as earlier in [1] by the experimental value of the films laser ablation destruction threshold energy density under the laser radiation pulse of 20 ns time duration F_{bn}, and the mechanical strength value was the composites microhardness H. The particle diameter of the sol dispersed phase was calculated by Heller method and the particles packing density in the layer value on the base of the on of light transmittance and viscosity measurements [3]. It has been stated that the particle size increasing appear in the reducing as the microhardness H and the F_{bn} values. However, the opposite phenomenon in the threshold energy and microhardness growth with the film thickness increasing has been obtained at the drawing velocity increasing up to 5.8 mm/s. The deviation of the sol particles forms from the pseudospherical and the sol to the substrate flow regime changing with the drawing velocity increasing may be mentioned among the most probable its causes. This work was partially financial supported by the Basic part of the Russian Federation Ministry of Education and Science State Task, project No. 2284 and RFBR grant, project No. 14-43-08049.

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The sols parameters influence on the optical properties of nanocomposites

Kaunov V S[@], Chartiy P V, Nartsev V M, Shemanin V G, Zakalova E Yu and Atkarskaya A B

Novorossiysk Polytechnic Institute of the Kuban State Technical University, Karl Marx 20, Novorossiysk 353900, Russia

[@] nvr10@mail.ru

The oxide films drawn on the glass surface by different methods are widely used to change the optical, mechanical and other properties of the glass samples. The significant influence on the glass composites properties has the state of the dispersed phase into the film-forming sol in the chemical method—sol-gel technology [1]. The viscosity η and the sols light transmission at the fixed wavelengths τ_λ, the refractive index n, thickness h, the threshold energy density of the laser ablation film destruction F_{bn} and F_{bm} and the composite microhardness H have been measured in experiments in the continuing studies in [2]. It was assumed that sol particle shape close to spherical in all of our calculations. Then the sols viscosity is proportional to the dispersed phase volume fraction φ [1]. The sol solid phase particle diameter d was calculated from the Heller equation [2] and the particles packing density into the film layer γ was assessed by [3]. Therefore, the laser beam after the thin film destruction comes in contact with a solid and infusible substrate and the laser ablation threshold energy increasing with the packing density decreasing in the film layer dispersed phase can be explained such a way. This work was partially financial supported by the Basic part of the Russian Federation Ministry of Education and Science State Task, project No. 2284 and RFBR grant, project No. 14-43-08049.

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Investigation of the effect of laser radiation on the dielectric properties of polymethylmetacrylate

Torshhoeva Z S[1,@], Ahriev A S[1], Kunizhev B I[2] and Kugotova A M[2]

[1] Ingush State University, Magistralnaya 39, Nazran, Ingushetia 386001, Russia
[2] Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia

[@] torshhoeva.zina@yandex.ru

The effect of laser radiation on the dielectric properties of polymethylmethacrylate (PMMA) at frequency of 50 kHz is studied over a wide range of temperatures. We have shown that the processing of the samples with laser radiation leads to substantial changes in the dielectric constant and dielectric loss tangent [1].
Changes in the dielectric constant and dielectric loss tangent, depending on the intensity of the laser radiation, the frequency of the external field, the temperature and time were investigated by dielectric loss. It was found that after two months after the laser irradiation of the dielectric constant of the samples of PMMA under the influence of relaxation processes at temperatures between 170 and 200 K is reduced to values of $\varepsilon' \sim 4$ of the original non-irradiated PMMA, and in the temperature range from 200 to 420 K dielectric constant has a value $\varepsilon' \sim 5.0$, higher than 30% of the permittivity starting unirradiated sample. The values of dielectric loss tangent $\tan\delta$ do not relax to values $\tan\delta$, corresponding to the original PMMA samples.

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On the mechanism of deep melting of targets under the action of high-power ytterbium fiber laser

Kochurin E A[1,@], Lisenkov V V[1,2], Osipov V V[1], Platonov V V[1] and Zubarev N M[1]

[1] Institute of Electrophysics of the Ural Branch of the Russian Academy of Sciences, Amundsen 106, Ekaterinburg 620016, Russia
[2] Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

[@] kochurin@iep.uran.ru

The present work is devoted to theoretical stability analysis of liquid melt in the crater of laser plume occurring in laser ablation of the yttrium oxide Nd^{+3}:Y_2O_3 targets. The influence of pulsed repetitive CO_2 laser and ytterbium-fiber laser on the targets was experimentally and theoretically studied in [1]. The experiments have shown, that the radiation of fiber laser leads to formation sufficiently deeper craters (depth $h_c \sim 150$–200 μm) than for the pulsed CO_2 laser ($h_c \sim 30$ μm) on the targets surface. Wherein the total energy of a pulse for two lasers was almost equal and was about 1 J.

In the present work, we study hydrodynamic processes in the crater occurring under the pressure of target vapor and tangential velocity jump between plasma moving upward and melted crater walls. Theoretical analysis has shown that hydrodynamic instabilities can arise at the molten walls of the crater. The wavelength of dominant mode (i.e. the scale of fastest growing perturbations) for the process discussed is about $\lambda_m \sim 20$–80 μm. Thus, the hydrodynamic shear instability can lead to an additional emission of target material in the liquid phase.

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Monitoring of the thermal melting of a silver surface layer with use of probing laser light

Batenin V M, Kachalov V V, Kourilovich A V and Mendeleyev V Y[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] v_mendeleyev@ihed.ras.ru

Optical monitoring of the thermal melting of materials caused by high power laser radiation uses the dependence of the reflectivity on the surface temperature. The reflectivity of the heated surface layer changes gradually and remains constant after the melting of the layer [1]. The thermal melting of the surface layer is considered as the nucleation followed by the nuclei coalescence. It cannot be detected using the reflectivity. In this article, the thermal melting of the surface layer is studied experimentally for silver samples by measuring temperature of the samples and registering patterns of probing laser light scattered and specularly reflected from the surfaces. The samples having unidirectional roughness were heated in an electric furnace. The study has helped clarify the following features of the patterns which allow detect the melting of the surface layer: presence of isotropic scattering during the nucleation; decline in the intensity of the unidirectional scattering as a sign of the roughness evolution; aberrations in shape of the specularly reflected laser light as a sign of spatial irregularity in the liquid phase; absence of changes in the shape of the reflected light as a sign of completion of the melting. Also we found a phenomenon similar to the directional crystallization [2]. A rod of silver grew out the molten silver against the direction of the laser beam.

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Multichannel scintillation spectrometer of pulse hard x-ray radiation using "shot through" geometry

Ignatiev N G, Ivanov M I, Krapiva P S, Nesterenko A O[@] and Svetlov E V

All-Russia Research Institute of Automatics named after Dukhov, Sushchevskaya 22, Moscow 127055, Russia

[@] radamat@rambler.ru

The report provides information about 8-channel scintillation spectrometer TSRI1.150 that has been developed at FSUE "VNIIA" and intended to dynamically measure parameters of hard x-ray radiation on laser and electrophysical facilities in the range of energy from 4 to about 500 keV. The spectrometer is based on photomultiplier with TNFT25-type microchannel plate with a photocathode 25 mm in diameter and a time resolution of less than 0.5 ns. The spectrometer uses a set of "fast" scintillators with appropriate edge filters. The filter-scintillator pairs are aligned in sequence (in "shot through" geometry) with effective thicknesses and atomic numbers increases with distance from source. Filters and scintillators are chosen so that the multiplication of filter transmission and scintillator efficiency functions gives nearly 100% transmission in chosen energy ranges, and almost completely passes radiation for the following pairs of filters and scintillators. The spectrometer uses three type of scintillators. First, PS-B2 made of polystyrol ($t_{0.5} = 0.7$ ns) thickness of 0.5 and 1.5 mm. Second, ZnO ($t_{0.5} = 0.5$ ns) thickness of 0.14, 0.3 and 0.54 mm. And third, BaF_2 ($t_{0.5} = 0.9$ ns) thickness of 0.6, 1.5 and 3.0 mm. Edge filters used foils of Ti, Cu, Zr, Sn, Gd, Pb and W thickness off from 15 to 300 μm. The spectrometer has two independent channels: the first one separates photons with average energies of 4.5, 17, 48 and 110 keV, the second one—with energies of 7.5, 25, 75 and 250 keV. Energy resolution of the channels is about 11 to 35%. Time resolution is no more than 1.5 ns.

Microchannel-plate based subnanosecond highly sensitive x-ray detector for diagnostic of high-speed processes in the plasma

Ignatiev N G, Ivanov M I, Korotkov K E, Krapiva P S, Moskalenko I N, Nesterenko A O, Svetlov E V and Zhukov P A[@]

All-Russia Research Institute of Automatics named after Dukhov, Sushchevskaya 22, Moscow 127055, Russia

[@] trigun.forever@gmail.com

We present the high-speed highly sensitive microchannel-plate (MCP) based x-ray detectors TDRI6 (1 MCP) and TDRI6-01 (2 MCP). The detectors are designed to measure the flux density of the x-ray radiation with energy (0.05–50) keV and pulse duration of 1 to 20 ns. Operating pressure of the detectors is less than 1×10^{-4} Torr. Open MCP plate with a Cr surface contact layer is used as an x-ray sensitive cathode. MCP plate diameter is 8 mm. Temporal resolution for both types of detectors, measured by femtosecond laser based x-ray source, is not more than 0.3 ns for both types of detector. The spectral response was investigated for x-ray energies from 0.1 to 10 keV on the x-ray calibration installation T20-L8. The maximum detectors sensitivity (for x-ray energy 0.28 keV) is 1×10^{-1} A cm^2/W for the detector TDRI6-01 and 1×10^{-4} A cm^2/W for the detector TDRI6. The sensitivity can be adjusted by using two mesh attenuators and by reducing the voltage on the MCP plates. The supply voltage for TDRI6-01 is 2 kV and for TDRI6 is 1 kV. The sensitivity adjustment range—more than 100. The maximum detectors line current is 0.5 A. The detectors dimensions (without cable and connectors): length—21 mm; width—14 mm; height—9 mm. As compared to silicon type x-ray detectors like an AXUV and SPPD11 the detectors TDRI6 and TDRI6-01 is more than two orders of magnitude more sensitive and have a higher speed.

The account of atmospheric turbulence in estimating path loss of near infrared laser radiation

Zaponov A E[@] and Sakharov M V

Military Academy of Strategic Rocket Troops after Peter the Great, Kitaygorodskiy 9, Moscow 109074, Russia

[@] nopaz@mail.ru

Laser technologies are actively used in aviation and space equipment today. For example, laser is used in distance Earth probing and monitoring of near-Earth space systems, network of specialized laser stations is created, which is the part of International Laser Ranging Service (IRLS). The power of lasers, which are used in these systems, is in the range from watts to kilowatts. Powerful lasers, which can be used in these systems, can interact with different aerial vehicles and devices on their boards. It can be harmful for some devices. That is why the task of estimating losses of laser radiation (LR) when passing the atmosphere, a significant impact on the value of which has turbulence, is actual. Method [1] of estimating the loss of near infrared (IR) LR of when passing the atmosphere was improved to account of the impact of the turbulence. Mathematical model of turbulence [2–4] was used for determination of divergence of LR on the route taking into account the turbulence. Test calculations were carried out in accordance with the proposed improved method. Analysis of the values in the last two columns of table 1 suggests, that the neglect of turbulence increases the flux density of LR on the receiver in about 6 times. Increasing the angle of the route, as well as reducing the distance between the source and receiver leads to an increase of flux density of LR on the receiver.

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Combined dc electric–ultraviolet and near infrared optical breakdown of Ar in a wide range of impact parameters

Loktionov E Yu[@], Pasechnikov N A and Telekh V D

Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] stcpe@bmstu.ru

Laser-induced electric breakdown has been investigated for a long time for radiation propagating collinearly to the electric field. This configuration has been used to facilitate conducting channel formation by partial ionizing of the gap. Orthogonal scheme is less investigated, but is of particular interest.

We have experimentally determined the breakdown thresholds of Ar and discharge plasma dynamics at 213–1064 nm irradiation by 18 ns and 71 ps laser pulses in the electric field up to 13.2 kV/cm and pressures of 6.7×10^2–5.5×10^5 Pa.

Different breakdown regimes and mechanisms are discussed according to the results obtained. Dense radiating plasma stagnation region formed due to optical and electric breakdown shock waves interference at certain conditions is demonstrated.

Dipole–dipole interactions between atoms in a partly excited resonance gas

Sautenkov V A

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

vsautenkov@gmail.com

Dipole–dipole interactions change the optical properties of dense resonance media. In the slightly excited media the dipole–dipole interactions were studied quite well. Situation in the strongly excited medium is still not clarified. In our presentation experimental studies of dipole–dipole interactions in partly excited resonance gases are discussed. By density the resonance gases can be defined as rarefied gases, where dipole broadening of atomic transitions is much less than Doppler width, and dense gases, where dipole broadening is much more than Doppler width. In theoretical work [1] the dipole–dipole interactions were analyzed in the frame of binary impact collisions, which is valid for the rarefied gases. Calculated dipole broadening should be independent on excitation. The theoretical results for the rarefied gases were confirmed by our experimental research [2]. In our recent publications the observations of reduction of dipole broadening in the excited dense gases have been reported [3]. This effect can be explained by homogeneous dipole broadening of atomic transitions in the dense gases when the interaction time during atomic collisions has to be taking into account. The measured spectral width is proportional to the ground state population [3]. A modified expression for optical response of the excited resonance gas is suggested.

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Ultraviolet pulse laser photosynthesis of binary metal-carbon nanoparticles

Eremin A V, Gurentsov E V, Mikheyeva E Yu and Musikhin S A[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] stasntsk@gmail.com

Metal nanoparticles show a growing interest due to their magnetic properties. Metal magnetic particles are expected to show higher performance than oxide ones in different applications because of their high saturation magnetization. A carbon shell over metallic core makes them resistant to oxidation and corrosion allows interacting with organic compounds. In this study, the uv laser photolysis of the mixtures containing different hydrocarbons and iron pentacarbonyl was implemented for binary iron-carbon nanoparticle formation. The energy source used for photo-dissociation of precursors was a pulsed Nd:Yag laser operated at a wavelength of 266 nm. Under uv radiation the molecules of $Fe(CO)_5$ have decomposed, forming the atomic iron vapor and unsaturated carbonyls at well-known and easily controllable parameters. The subsequent condensation of supersaturated metal vapor resulted in small iron clusters and nanoparticles formation. The growth process of the nanoparticles was observed by a laser light extinction method. Additionally nanoparticle samples were investigated by a transmission electron microscope. The particle sizes were measured by statistical treatment of microphotographs. The elemental analysis by energy-dispersive x-ray spectroscopy and electron diffraction pattern gave the composition and the structure of nanoparticles. The core-shelled iron-carbon nanoparticles formation was observed in the joint laser photolysis of iron pentacarbonyl with benzene and acetylene. The photolysis of the toluene, butanol and methane mixtures with iron pentacarbonyl revealed in the pure iron particles formations which were fast oxidized in air when extracted out of the reactor. This work was supported by the Russian Science Foundation (project No. 14-50-00124).

Electronic and spatial structure features of calibrated gold clusters

Erenburg S B[1,2], Trubina S V[1,@], Kovalenko E A[1], Geras'ko O A[1], Zaikovskii V I[3] and Kvashnina K O[4]

[1] Institute of Inorganic Chemistry of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 3, Novosibirsk 630090, Russia
[2] Budker Institute of Nuclear Physics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 11, Novosibirsk 630090, Russia
[3] Boreskov Institute of Catalysis of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 5, Novosibirsk 630090, Russia
[4] European Synchrotron Radiation Facilities, Avenue des Martyrs 71, Grenoble 38043, France

[@] svt@niic.nsc.ru

On passing from a bulk solid to 10 nm sizes and less, small particles exhibit new or essentially modified properties: crystal lattice parameters, electronic structure, magnetic, optical, and catalytic properties, and surface morphology change. In particular, it is stated that finely dispersed metals are often active in the reactions in which bulk metals are either weakly active or passive at all. The AuL_3 XAFS spectra have been measured for samples containing calibrated gold nanoparticles with diameter less than 1nm in cavities of cucurbituril molecules (CB[6, 7]). The local structural parameters and electronic structure peculiarities of particles were determined by EXAFS and XANES spectroscopy using synchrotron radiation. It has been found that gold clusters are characterized by smaller (less than 0.03 Å) interatomic distances as compared with bulk gold. No visible shifts of AuL_3 absorption edges and differences in the Au charge state for Au[6, 7] samples containing small Au clusters were detected in comparison with bulk Au metal. A threefold and more increase in the Debye-Waller factor at 12 K was found for the nanoparticles in comparison with bulk metal and correspondingly, a substantial increase in the structural disorder. It has been found that special chemical (catalytic) and physical (optical) properties of small gold particles are likely to be attributed to this structure changes and the size effect with the appearance of a band gap between the occupied and unoccupied electronic states.

Spatial and electronic structure of GaN/AlN and Ge/Si multilayered heterosystems

Erenburg S B[1,2,@], Trubina S V[1], Zhuravlev K S[3,4], Malin T V[3], Zinovyev V A[3], Dvurechenskii A V[3,4], Kuchinskaya P A[3] and Kvashnina K O[5]

[1] Institute of Inorganic Chemistry of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 3, Novosibirsk 630090, Russia
[2] Budker Institute of Nuclear Physics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 11, Novosibirsk 630090, Russia
[3] Rzhanov Institute of Semiconductor Physics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 13, Novosibirsk 630090, Russia
[4] Novosibirsk State University, Pirogova Street 2, Novosibirsk 630090, Russia
[5] European Synchrotron Radiation Facilities, Avenue des Martyrs 71, Grenoble 38043, France

[@] simon@niic.nsc.ru

III-nitride heterostructures in the form of multilayered quantum wells (MQWs) or quantum dots (QDs) are promising candidates for high-speed intersubband optical devices relying on the quantum confinement of electrons. The systems with interacting QDs—molecules (in particular, GeSi nanorings or quantum rings) have attracted much attention both as ground for studying coupling and energy transfer processes between "artificial atoms" and a new systems, which substantially extend the range of possible applications of QDs. Interatomic distances, coordination numbers and Debye–Waller factors were determined by means of EXAFS spectroscopy and the relationship between the variations in these parameters and the morphology of superlattices and QDs symmetric assembles were established. The EXAFS technique has been used to study the local structure of thin hexagonal GaN/AlN MQWs grown by ammonia MBE at different temperatures. It is shown that the heterointerface intermixing leads to a decrease in the Ga-Al interatomic distance and the Ga-Ga coordination number in MQWs.
The work is supported by the RFBR grant 16-02-00175.

Microwave assisted creation of selenium polymeric nanomaterials

Savintsev Yu P[@], Shevchenko V S and Urakaev F Kh

Sobolev Institute of Geology and Mineralogy of the Siberian Branch of the Russian Academy of Sciences, Akademika Koptyuga 3, Novosibirsk 630090, Russia

[@] savincev1940@mail.ru

Selenium nanomaterials still attract attention of many scientists of the world. These substances have numerous applications. So recently technology of production of inexpensive solar cells with help of microwave treatment on the base of selenium nanoparticles was created. But the very promising applications of selenium containing polymeric materials are on the field of nanobiomaterials creations. These are such very interesting systems for nanobiotechnology as self-assembled substances with unique redox properties, when the same species can have oxidative and reductive properties, systems, working as gene delivery vehicles. In this research we try to find way to obtain long living polymeric systems with selenium nanoparticles. Microwave treatments were used on different steps of synthesis, which involve mixing of solutions of polymer, surfactant, selenous acid and sulfur dioxide. Films of nanocomposites, produced after drying its water solutions were investigated by optical and electronic microscopy, x-ray, uv-vis spectroscopy. Conclusions were made on the structure and stability of obtained systems.

Diffusion mass transfer in multicomponent multilayered metallic samples irradiated by high-current electron beams

Leyvi A Ya[2,@], Pridannikov A V[1], Talala K A[1,2], Khlybov V I[1] and Yalovets A P[2]

[1] Open Joint Stock Company "Academician Makeyev State Rocket Centre", Turgoyakskoye Shosse 1, Miass, Chelyabinsk Region 456300, Russia
[2] South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia

[@] ktalala@yandex.ru

Nowadays the treatment of materials with intensive energy flows (electron and ion beams, plasma, laser emission) is widely used to modify properties of a material. The mass transfer processes are important for the formation of the material new properties. In systems of thin (less than 10 μm) films diffusion is a key mechanism of the mass transfer. Authors developed software to compute the diffusion mass transfer in multicomponent multilayered samples exposed to a high-current electron beam or a flow of plasma with consideration for melting and evaporation. We considered the possibility to apply different metallic layers gradually exposed to the electron beam one by one. The Ti-Zr-Fe system was estimated and optimum application and treatment modes for increased wear-resistance were defined.

Experimental studies of shock wave generation in porous composites under pulse electron beam

Dan'ko S A[1], Demidov B A[1], Efremov V P[2], Kalinin Yu G[1], Kazakov E D[1,@], Kurilo A A[1] and Strizhakov M G[1]

[1] National Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] evgenische@gmail.com

Studies of constructional material behavior under pulse power densities are very important both for fundamental researches and different applications. Modeling of shock wave generation in porous composites is complicated task because of complex structure of such materials. It is necessary to have rather detailed experimental database for verification of these models. In this paper we present experiments that were carried out on high current electron accelerator "Calamari". This facility provides energy flux in the range 10–10^3 J/cm^2 for electron energies of 120–350 keV [1]. Beam duration is 100 ns. In our experiments we irradiated porous composite targets with density 0.1–0.8 g/cm^2. The electron range in these materials was at least 1.5 mm. In the hole of irradiated targets volume explosion was observed. The beam current was measured by noninductive shunt, the electron energy was calculated from measured diode voltage, the square of energy output was measured by hard x-ray pinhole camera for high energy radiation [2]. Plasma expansion was registered in visible range by streak camera. Irradiated targets were investigated by electron microscope.

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Study of plasma implosion dynamics in condensed deuterated Z-pinch on the Angara-5-1

Aleksandrov V V[1], Frolov I N[1], Grabovskiy E V[1], Gritsuk A N[1], Ivanov M I[3,@], Kalinin Yu G[2], Kazakov E D[2], Korolev V D[2], Lauhin J I[1], Medovshchikov S F[1], Mitrofanov K N[1], Oleinik G M[1], Pimenov V G[5], Smirnova E A[2] and Volobuev I V[4]

[1] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 142190, Russia

[2] National Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia

[3] All-Russia Research Institute of Automatics named after Dukhov, Sushchevskaya 22, Moscow 127055, Russia

[4] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

[5] Zelinsky Institute of Organic Chemistry of the Russian Academy of Sciences, Leninsky Avenue 47, Moscow 119991, Russia

[@] ivanov3575@yandex.ru

The implosion dynamics of condensed deuterated Z-pinch were studied on the installation Angara-5-1 with a current of up to 3.5 kA with time of increase of 100 ns. For implication of effect of a energy focusing central part of load were made from deuterated polyethylene with density of 0.1–0.4 g/cm^3 and a diameter of 1–3 mm. Spatial–time parameters of plasma in Z-pinch were investigated by a diagnostic set of the Angara-5-1, which includes time-frame photography in soft x-ray and VUV spectral region, an optical streak camera, time integrated of three pinhole cameras, soft x-ray pin-diodes and vacuum photoemission detectors. Energy characteristics of neutron emission were determined by means of time-of-flight method. Neutrons were detected with the help of four scintillation detectors, placed along the Z-pinch axis and normally to axis. The total neutron yield was measured by activation detectors. To be continued...

Numerical methods of the current pulse restoration according to the penetration rate of electric field induced inside the tube

Khirianova A I[1,@] **and Tkachenko S I**[1,2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] khirianova.alexandra@gmail.com

To numerical study the model of the coaxial part of magnetically insulated transmission line under extreme thermal and dynamic impact we need to restore the current pulse. The problem of restoration of the current pulse, flowing through the tube (with the walls considerably thicker than skin layer), is solved. For this purpose we make mental division of a thick tube into the series of a thin tubules (their thickness should be comparable to the skin depth). Solving of the diffusion equation of magnetic field for each tubule provides the connection of the magnetic field for the internal and external surfaces of the tubules; using the theorem on the circulation of the magnetic field, we get the current flowing through the tube. For the calculation of boundary conditions for the innermost tubule we used the electric field intensity measured on the inner surface of the tube.

The method takes into account inhomogeneity of the tube heating and consequently, the changing of matter conductance over thickness tube and time. The algorithm verification been performed for test problems, as well as at the comparison with the experimental data. The calculation results are in good agreement with the experimental data.

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Similarity in exploding wires simulated by molecular dynamics and smoothed particle hydrodynamics

Egorova M S[1,@], Tkachenko S I[2,3], Dyachkov S A[1], Parshikov A N[1] and Zhakhovsky V V[1]

[1] All-Russia Research Institute of Automatics named after Dukhov, Sushchevskaya 22, Moscow 127055, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
[3] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] egorova.maria.serg@gmail.com

High-resolution x-ray radiography indicates that a complex small-scale structure is formed inside an exploding wire. It was recently shown in molecular dynamics (MD) simulation [1] that such a structure can be formed via cavitation of liquid metal during expansion of heated aluminum cylinders with radii up to 200 nm. The initial stage with electric current heating and magnetic confinement of wire material was modeled by our magnetohydrodynamic code. The obtained wire radius and material state at current cutoff resulting in magnetic pressure drop were used as initial data for MD simulation. To validate MD results for micrometer-sized wires used in experiments we employ smoothed particle hydrodynamics (SPH) [2] for aluminum wire with the equation of state and tensile strength derived from MD simulation. We demonstrate that such consistent MD and SPH simulations give similar expansion dynamics of exploding wire. Moreover, the density and velocity profiles obtained from MD simulation of nanometer-sized wires and SPH modeling of micrometer-sized wires are scaled well. Both methods provide similar evolution of exploding wire, including cavitation of central part and formation of outward liquid shell, clearly visible on the high-resolution x-ray radiography images.

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Accurate determination of the inductive contribution to the voltage across a specimen in the pulsed Joule heating experiments

Kondratyev A M[@] and Rakhel A D

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] cpl593h@mail.ru

Pulsed Joule heating techniques are frequently used to study the properties of electrically conductive materials at high temperatures and pressures. A specimen in the form of a foil strip or thin plate is sandwiched between two plates of window material (sapphire or silica glass) and resistively self-heated by an electric current pulse of 10–100 kA magnitude and a rise time of less than one microsecond. The geometrical dimensions of the specimen are chosen so that the heating is uniform and thermal expansion of the specimen is nearly one-dimensional. Current through the specimen and voltage drop across it are measured during such an experiment as functions of time. From the measured quantities the Joule heat dissipated in the specimen and its resistance can be determined. Due to the high velocity of the current variation a significant EMF is induced in the voltage-measuring circuit. In order to determine the active component of the voltage across the specimen the EMF must be subtracted from the measured voltage signal. In present work a method is reported that allows this subtraction to be done with reasonable accuracy. We show that using this method, the measured heat of fusion of tungsten, graphite, and the latent heat of the transition from alfa to beta phase of zirconium are consistent with the most accurate literature data.

On the possibility of application the deformation induced defects in ^{29}Si for cubit technology

Steinman E A[1,@], Morgunov R B[2], Koplak O V[2] and Tereschenko A N[1]

[1] Institute of Solid State Physics of the Russian Academy of Sciences, Institutskaya Street 2, Chernogolovka, Moscow Region 142432, Russia
[2] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] steinman@issp.ac.ru

Paramagnetic defects of new kinds are obtained as a consequence of plastic deformation of isotopically enriched ^{29}Si. A correlation of temperature behavior of dislocation luminescence lines and the magnetic susceptibility was found experimentally. The electron paramagnetic resonance (EPR) spectra are anisotropic and have a considerable width (up to 1 kOe). Nonuniform broadening of EPR bands is determined by variations of internal magnetic field in the correlated defect clusters. The nuclear magnetic resonance (NMR) spectra of the deformed crystals are Pake doublets splitted by spin-spin nuclear interaction. The broadening of NMR spectra is caused by a dipole–dipole relaxation.

Dislocation structures in oxide nuclear fuel: Computer simulation and experiments

Lunev A V[1,2,@], Baranov V G[2], Isaenkova M G[2] and Krymskaya O A[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

[@] AVLunev@mephi.ru

In nuclear fuel based on uranium dioxide, dislocations are created both by radiation damage and by warm deformation. The build-up of dislocation density in UO_2 can be rather significant allowing plastic flow to control some of the most important processes during fabrication and operation of this fuel. However, very little is known yet about the accumulation and interaction of dislocations in oxide nuclear fuel. Most model predictions are based on rate theory, which might not reproduce the intrinsic mechanisms correctly. At the same time, a consistent experimental study requires representative sampling, which in case of in-pile tests could hardly be achieved. Present research focuses on a combination of experimental techniques (x-ray diffraction, atomic-force microscopy) and computer simulation (2D dislocation dynamics) to study dislocation structures in irradiated/deformed UO_2. Results reveal that in response to external action the density of chaotically distributed dislocations in UO_2 increases, which in case of enhanced diffusion leads to self-organization processes producing a periodic structure of dislocation walls at high damage dose/degree of deformation. The results should be used to develop advanced performance codes for oxide nuclear fuel in power reactors.

Molecular dynamics simulation of primary radiation damage in Fe-Cr alloy

Zolnikov K P[@], Korchuganov A V and Kryzhevich D S

Institute of Strength Physics and Material Science of the Siberian Branch of the Russian Academy of Sciences, Akademicheskii 2/4, Tomsk 634021, Russia

[@] kost@ispms.tsc.ru

The simulation of the atomic displacement cascades generated by radiation in the iron-chromium alloys on the basis of the molecular dynamics method was carried out. Interatomic interactions were described on the base of the Finnis-Sinclair approximation. Used potentials allowed describing with high accuracy many mechanical and physical properties which are very important for the atomic displacement cascade simulations. The simulated crystallites had a parallelepiped shape. The periodic boundary conditions in all directions were used at displacement cascade simulations. Atomic displacement cascades were generated by the primary knock-on atom, which energy varied from 1 to 20 keV. The number of atoms in the simulated crystallite varied from 500000 to 2500000 depending on the primary knock-on atom energy. The simulation of the dynamics of atomic displacement cascades and the calculation of the cascade parameters (durations of the main stages, the size of the radiation-damaged region, defect production efficiency) in the iron-chromium alloy for different energies of primary knock-on atom were made. Sizes of formed point defect clusters and their distribution in the crystallite volume were calculated. Radiation damage in iron-chromium alloy caused by generation and evolution of cascades of atomic displacements based on the analysis of spatial and quantitative distribution of the generated point defects and their clusters was studied.

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Comparison of pulsed cathodoluminescence spectra of LFS crystals, doped by different elements, before and after gamma-irradiation

Kozlov V A[1], Kutovoi S A[2], Pestovskii N V[1,3,@], Petrov A A[1,3], Savinov S Yu[1,3], Zagumennii A I[2], Zavartsev Yu D[2] and Zavertiaev M V[1]

[1] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia
[2] Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova 38, Moscow 119991, Russia
[3] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] pestovsky@phystech.edu

Pulsed cathodoluminescence (PCL) spectra of $Lu_{2+2y}Si_{1+y}O_{5-y}$ (LFS) crystal, co-doped by Ca^{2+}, Sc^{3+}, Y^{3+}, Yb^{3+}, Ce^{3+} ions before and after the gamma-irradiation, produced by the ^{60}Co source is studied. PCL spectra of samples had been compared before and after the gamma-irradation at dose 45 Mrad. It is shown that PCL spectra of samples LFS:Sc, LFS:Yb, LFS:Sc:Yb are exposed to significant radiation degradation at doses of 45 Mrad. PCL spectra of sample LFS:Sc:Y:Ce:Ca has no difference before and after the gamma-irradiation with doses of 45 Mrad. This study was financially supported by the Russian Science Foundation (project No. 14-22-00273).

Investigation of cation impurities diffusion in Al_2O_3: The effect of cation size and valence

Kislenko S A[@], Vlaskin M S and Zhuk A Z

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] kislenko@ihed.ras.ru

Atomistic simulation based on energy minimization techniques was used to study the vacancy diffusion mechanism of impurities with different sizes and valences in corundum (α-Al_2O_3): Mg^{2+}, Co^{2+}, Fe^{2+}, Cd^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Cr^{3+}, Ga^{3+}, Fe^{3+}, Sc^{3+}, In^{3+}, Yb^{3+}, Y^{3+}, Sm^{3+}, Rh^{4+}, Ti^{4+}, Ru^{4+}, Mo^{4+}, Sn^{4+}, Pu^{4+}. It was employed the Born model of an ionic crystal with account of the electronic polarizability of oxygen ions. The migration energies of the impurities for different possible migration paths were obtained by the nudged elastic band method. Binding energies of an impurity-aluminium vacancy pair were also estimated. It was shown that two paths give the main contribution to vacancy diffusion: migration along C axis through an octahedral interstitial site formed by oxygen ions, and jumps to the nearest aluminium sites. Migration energy of isovalent impurities weakly depends on ion size. Simulation revealed the divacancy mechanism of diffusion for divalent impurities mediated by defect clusters containing simultaneously oxygen and aluminium vacancies.

Molecular dynamic simulation of influence of cathode morphology on cathode/electrolyte interface

Pavlov S V[1,2,@] **and Kislenko S A**[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] sergey.v.pavlov@phystech.edu

The influence of the cathode morphology on the structure of cathode/electrolyte interface is investigated by molecular dynamic simulation. Acetonitrile is chosen as electrolyte, and three configurations of cathode are studied: graphite with parallel and perpendicular orientation of basal planes with respect to the interface plane, and single graphene nanosheet. Density distribution of electrolyte near cathodes is obtained, and the study revealed the influence of cathode configuration on the structure of cathode/electrolyte interface. The potential of mean force for lithium ion near the cathode planes is calculated. The simulation shows that local density of electrolyte correlates with potential of mean force. Based on the results of simulations we propose the hypotheses which explains increased efficiency of the oxygen reduction reaction at the edge of graphene.
The work was supported by grant from the Russian Science Foundation (project No. 14-50-00124).

Positron creation in the air at powerful streak lightning: Substantiation of ball lightning positron nature

Boriev I A

Institute of Energy Problems of Chemical Physics of the Russian Academy of Sciences, Leninsky Avenue 38 Corps 2, Moscow 117829, Russia

boriev@binep.ac.ru

Positron creation in thunderclouds at streak lightning was revealed in 2009 using space telescope Fermi. Then creation of electrons and gamma quanta with MeV energy was found. Their creation is due to high electric fields (up to 200 MV) in thunderclouds what generate powerful streak lightning (with up to $\sim 10^{21}$ high energy electrons), which often generate ball lightning. Positrons appear at electron-positron pair creation (from dark matter, which fills space) under action of bremsstrahlung gamma quanta produced at retardation of electrons in atomic electric field of air molecules.
Assumption that ball lightning is a bunch of many (up to $\sim 10^{17}$) positrons explains all observed specific properties of ball lightning [1]. Confluence possibility of positrons is possible for concurrently and next to created positrons from nearest dark matter. If around created positrons will be not dark matter (to produce their electric fields causing their repulsion), then positrons, as identical material vortex, may confluence in one rotating bunch. According to energy conservation law the rotation speed of growing positron bunch must slow down so that its surface speed stays constant [1]. Hence electric field of positron bunch (due to polarization by its rotation of around dark matter) will stay constant and small, as it is observed.

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Parameters of powerful explosive for redirection of the asteroid Apophis to the Moon surface

Ostrik A V[@] and Fortov V E

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] ostrik@ficp.ac.ru

The problem aiming qualitative change of an Apophis orbit when its movements in Solar system comes to an end is formulated in [1, 2]. Instead of passive saving tactics the variant of use of this asteroid is considered for realization of large-scale space experiment. This experiment is shock interaction of an asteroid and the Moon. The organization of space scale collision will allow to solve a set of the physical questions concerning the Moon [2].

Correction of an Apophis orbit on July 22, 2016 or on July 11, 2017 by means of making of an speed increment 7.33 m/s for an asteroid is sufficient. As result of calculations by method [3] this correction provides Apophis redirection to the Moon surface.

Superficial and near-surface explosions lead to asteroid fragmentation that is undesirable for a set of reasons. The variant of the outlying explosion is more preferable. Results of calculations show that the speed increment 10 m/s is realized at the power of outlying explosion about 10–40 Mt TTN. It depends on distance before explosion (50–100 m), thermodynamic properties of Apophis material and its porosity. In case of outlying explosion the basic factor is mechanical action of x-ray and neutron fluxes [4]. We used Planck spectrum for estimates of mechanical radiation action.

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Requirements to admissible defects of new generation sheetings

Bugay I V[1,@] and Ostrik A V[2]

[1] Institute of Applied Mechanics of the Russian Academy of Sciences, Leninsky Avenue 32a, Moscow 117334, Russia
[2] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] ibug@mail.ru

Protection of constructions from thermal and mechanical actions of the ionizing radiation (IR) by means of the heterogeneous coverings (HC) having structure represents considerable practical interest [1]. Calculation methods and numerical codes are developed for determination of parameters of mechanical IR action formed on HC [2]. Results of investigations are given in the present work.
The main attention is paid to heterogeneous materials having properties gradient along HC thickness. For gradient sheetings the process of making of the decreasing or increasing gradient of filler concentration is the most technological. Tin dioxide and cerium fluoride and lead and microsphere (continuous and hollow, metalized and not metalized) are considered as filler at research of protective properties for such HC.
Influence of different types of HC defects on parameters of mechanical IR action is investigated. It is shown on the basis of the analysis of settlement and experimental data that deviations in sizes and a form and the mass content of disperse inclusions are defining. Besides it is established that deviations in sizes and the mass contents should not exceed 20 and 10% respectively. Influence of a deviation of filler form depends on sheeting type. The quantitative estimation of this influence demands further researches.

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Nuclear DD fusion in the potential well of a virtual cathode

Oginov A V, Kurilenkov Yu K[@], Karpukhin V T, Samoylov I S and Shpakov K V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] kurilenkovyuri@gmail.com

Processes of nuclear burning of various elements in the scheme of a compact inertial electrostatic confinement [1] implemented on the basis of a nanosecond vacuum discharge (NVD) with low-energy hollow cathode were investigated experimentally earlier [2, 3]. This paper presents the results of a recent series of DD fusion experiments on the anew created experimental stand NVD-2 combined with x-ray and neutron yield diagnostics. The voltage–current (V-A) characteristics of the discharge, the implemented experimentally regimes of generation of x-ray and DD neutrons are presented and discussed. The experimental results are compared with the results of particle-in-cell simulation of the nuclear DD fusion processes in NVD using electrodynamic code KARAT [3]. Recent series of DD fusion experiments on the new created experimental stand NVD-2 have reproducing in time-of-flight scheme the basic features of DD neutrons yield observed earlier [2, 4]. Meanwhile, the analysis of V-A characteristics and anode erosion shows that efficiency of energy deposition at initial stage of discharge is still insufficient. At present time, the ways to optimize the electrophysical processes at NVD-2 are clarified.

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Particle-in-cell modeling of p+^{11}B burning in the potential well of a virtual cathode

Kurilenkov Yu K[@], Tarakanov V P and Gus'kov S Yu

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] kurilenkovyuri@gmail.com

The neutron-free reaction of proton–boron nuclear burning accompanied with the yield of three alpha particles ($p + {}^{11}B \rightarrow \alpha + {}^{8}Be \rightarrow 3\alpha$) is of great fundamental and applied interest [1] which is growing permanently (see [2,3] and references therein). The present particle-in-cell (PIC) modeling of $p + {}^{11}B$ burning in the scheme of inertial electrostatic confinement [1] based on nanosecond vacuum discharge (NVD) [4] using code KARAT is carried out in the axially symmetric approximation (as it have been done earlier for modeling of DD syntheses at NVD [4]). Evolutions of the voltage at the coaxial inlet and the voltage between the anode and the virtual cathode (VC) are calculated. Boron ions and protons are accelerated in the potential well (PW) of VC in the direction of the axis, where their density and energy of head-on collisions are increasing, which actually leads to the appearance of alpha particles [5]. PIC modeling have recognizing that transfer to almost pure cylindrical geometry of cathode allows to optimize some of the key parameters of nuclear $p + {}^{11}B$ burning at PW of VC in NVD, and allow to hope on increasing of burning efficiency at the future NVD experiment.

This work is supported by grant No. 14-50-00124 from the Russian Science Foundation.

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Experimental modeling of lightning strike in soil

Fortov V E, Smirnov V P, Son E E, Bykov Yu A, Grabovskiy E V, Gribov A N, Oleinik G M and Saveliev A S[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] fisteh@mail.ru

Since 2010 in collaboration with the Federal Grid Company (JSC FGC UES) and the Krzhizhanovsky Power Engineering Institute we have started the investigation of the process when the lightning current goes through the soils. This problem appears in the energy industry and can affect on electrical energy delivery to consumers. The conductivity of soil and physical processes that occur during lightning strike can impose additional requirements on the grounding system of objects of electrical grid system. In Russian Federation the importance of this effect rises because of variety of soil types with conductance that can vary in several orders. Experimental modeling of the process can be carried out in laboratory or in the conditions that correspond to the real process (experiments at the field). To provide investigations the second way has been chosen and the special mobile laboratory with high voltage generator (HVG) that can operate independently was made. The scheme HVG is based on Arkadiev–Marx generator and generates the amplitude of voltage 2 MV (high impedance load), more than 50 kA of current (low impedance load) and the time profile of current is similar to that of lightning current. During the electrical discharge mobile laboratory registers the oscillograms of current, electrical potential difference between electrodes buried in soil, potential distribution on the ground surface, magnetic field strength near the surface and the high speed imaging of surface is carried out in order to detect sparks near test area. The work is devoted to experiments that carried out at Moscow region near the Troitsk where the soil has relatively low resistance. The study was performed by a grant from the Russian Science Foundation (project number 14-50-00124).

Development and optimization of a two-stage gasifier for heat and power production

Zaichenko V M and Kosov V V[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] kosov@ihed.ras.ru

The major methods of biomass thermal conversion are combustion in excess oxygen, gasification in reduced oxygen, and pyrolysis in the absence of oxygen. The end products of these methods are heat, gas, liquid and solid fuels. From the point of view of energy production, none of these methods can be considered optimal. A two-stage thermal conversion of biomass based on pyrolysis as the first stage and pyrolysis products cracking as the second stage can be considered the optimal method for energy production that allows obtaining synthesis gas consisting of hydrogen and carbon monoxide and not containing liquid or solid particles. On the base of the two stage cracking technology, there was designed an experimental power plant of electric power up to 50 kW. The power plant consists of a thermal conversion module and a gas engine power generator adapted for operation on syngas. Purposes of the work were determination of an optimal operation temperature of the thermal conversion module and an optimal size of pyrolysis products cracking chamber. Experiments on the pyrolysis products cracking at various temperatures show that the optimum cracking temperature is equal to 1000 °C. The maximum of syngas volume at this temperature is up to 1.5 m^3 per 1 kg of wood biomass. From the results of measuring the volume of gas produced in different mass ratios of charcoal and wood biomass processed, it follows that the maximum volume of the gas in the range of the mass ratio equal to 0.5–0.6.

Scientific bases of biomass processing into basic component of aviation fuel

Kachalov V V[1], Lavrenov V A[1,@], Lishchiner I I[1], Malova O V[1], Tarasov A L[2] and Zaichenko V M[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Zelinsky Institute of Organic Chemistry of the Russian Academy of Sciences, Leninsky Avenue 47, Moscow 119991, Russia

[@] v.a.lavrenov@gmail.com

A combination of feedstock pyrolysis at 600–700°C and the cracking of the volatile pyrolysis products on the charcoal at 1000°C allows to obtain a synthesis gas which contains 90% (vol.) or more of carbon monoxide (CO) and hydrogen (H_2) in approximately equal proportions. Such a synthesis gas contains no tar and its calorific value is 10–12 MJ/Nm^3.

Basic component of aviation fuel was synthesized in a two-stage process from gas obtained by pyrolytic processing of biomass. Methanol and dimethyl ether can be efficiently produced in a two-layer loading of methanolic catalyst and γ-Al_2O_3. The total conversion of CO per pass was 38.2% using for the synthesis of oxygenates a synthesis gas with adverse ratio of $H_2/CO = 0.96$. Conversion of CO to CH_3OH was 15.3% and the conversion of CO to dimethyl ether was 20.9%. A high yield of basic component per oxygenates mass (44.6%) was obtained during conversion. The high selectivity of the synthesis process for liquid hydrocarbons was observed. An optimal recipe of aviation fuel "B-92" based on a synthesized basic component was developed. The prototype of aviation fuel meets the requirements for "B-92" when straight fractions of 50–100°C (up to 35% wt.), isooctane (up to 10% wt.) and ethyl fluid (2.0 g/kg calculated as tetraethyl lead) is added to the basic component.

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Comparison of thermal conversion methods of different biomass types into gaseous fuel

Larina O M[@], Sinelshchikov V A and Sytchev G A

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] umnova.olya@gmail.com

Progress and adoption of distributed energy resource systems gave rise to the increased interest in the development of modern technologies of using renewable hydrocarbon resources for energy purposes. Biomass is quite universal type of the energy raw material that can be used either as a solid fuel for direct combustion, or as a raw material for obtaining liquid and gaseous fuels. Thermal methods of biomass conversion into gaseous fuel depending on the ways of generating the heat required for processing and the technique of putting the heat into feedstock can be divided into autothermal and allothermic. The former include the different schemes of gasification in which heat is produced by the partial combustion of raw material in controlled oxidizing atmosphere and the conversion of raw material into gas state occurs in the flow of combustion products. The latter include the pyrolysis methods in which heating of the feedstock is carried out in oxygen free environment. As a result, gas, liquid and solid products whose composition and mass depend on the final temperature and the heating rate are obtained. In the paper a comparison of the gas mixtures characteristics (volume, composition and calorific value) that can be obtained by different thermal conversion methods from the main biomass types is presented. The merits and demerits of these methods are discussed. From submitted data it follows that the two-stage pyrolysis technology, which consists of the biomass pyrolysis and the consequent high-temperature conversion of pyrolysis gases and vapours into synthesis gas by filtration through a porous carbon medium, allows to achieve both a high degree of biomass conversion into gaseous fuel and a high energy efficiency.

Challenges and opportunities of torrefaction technology

Kuzmina J S, Sytchev G A[@] and Zaichenko V M

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] george.sytchev@gmail.com

Since the active exploitation and usage of classical non-renewable energy resources the most promising direction is the development of technologies of heat and electricity production from renewable sources–biomass. This is important in terms of reducing the harmful man-made influence of fuel-and-energy sector on the ecological balance. One of the most important aims when using biomass is its pre-treatment. The paper describes the fuel preliminary preparation for combustion with such technological process as torrefaction. Torrefaction allows bringing the biomass fuel as close as it possible to fossil coals for the main thermotechnical parameters. During torrefaction moisture is removed from initial material and the partial thermal decomposition of its components appears. The final torrefied product can be recommended for utilization in existing coal-fired boilers without their major reconstruction. Thus torrefaction technology enables the partial or complete replacement of fossil coal. At JIHT RAS a torrefaction pilot plant is developed. As heat transfer medium the gas-piston engine exhaust gases were used. Results of researching and proposals for further development are showed in this paper.

Energy production estimation for Kosh-Agach grid-tie photovoltaic power plant for different photovoltaic module types

Gabderakhmanova T S[1,@], Kiseleva S V[2], Frid S E[1] and Tarasenko A B[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Lomonosov Moscow State University, Leninskiye Gory 1, Moscow 119991, Russia

[@] tts_91@mail.ru

According to the Russian Federation Government Resolution N 449 of May 28, 2013 capital expenses for photovoltaic (PV) grid-tie power plant from 5 MW (peak) can be compensated to owner in case he wins competition for renewable energy generation which is held by Russian Energy Ministry. Low capital expenses and large share of made-in-Russia components (at least 70% from 2016 are required) are important conditions to win the competition. PV modules are the most important components of PV plant that define its energy production, lifetime, demanded area and costs. So proper module choice is very important from the further PV plant operation. This paper is devoted to calculation of yearly energy production, demanded area and capital costs for first Russian 5 MW grid-tie PV plant in Altay Republic that is named KoshAgach. Simple linear calculation model, involving average solar radiation and temperature data, grid-tie inverter power-efficiency dependence and PV modules parameters is proposed. Monthly and yearly energy production, equipment costs and demanded area for PV plant are estimated for mono-, polycrystalline and amorphous modules. Calculation includes two types of initial radiation and temperature data such as average day for every month from NASA SSE and typical meteorology year generated from average data for every month. The peculiarities for each type of initial data and their influence on results are discussed.

4. Physics of Low Temperature Plasma

Interaction of laser radiation with shock-compressed strongly coupled plasma

Zaporozhets Yu B[1,@], Mintsev V B[1], Reinholz H[2] and Röpke G[2]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[2] University of Rostock, Universitätsplatz 3, Rostock 18051, Germany

[@] yubz@icp.ac.ru

Understanding the physics of strongly non-ideal plasmas requires a quantum statistical theory which adequately describes the behavior of strongly interacting charged particles since it plays a crucial role in such environments. The correct treatment of dissipative processes in such systems is possible only on the basis of sufficient information on the transport properties of the medium.

The results of new experiments on reflectivity of polarized light on explosively driven dense xenon plasma are presented. The study of polarized reflectivity properties of strongly correlated dense plasmas have been carried out simultaneously for s- and p-polarization using laser light of frequency $\nu_{\text{las}} = 2.83 \times 10^{14}$ s^{-1} ($\lambda_{\text{las}} = 1064$ nm) at incident angles up to $\theta = 30$. With density up to $\rho = 1.8$ g/cm^3, pressures up to $P = 9$ GPa and temperatures up to $T = 30000$ K of the investigated plasma, conditions with strong Coulomb interaction (the nonideality parameter up to $\Gamma = 1.6$) were present.

The thermodynamic parameters and composition of plasma were determined from the measured shock wave velocity with suitable calculations carried out. Working with a grand canonical ensemble, virial corrections have been taken into account due to charge-charge interactions (Debye approximation). Angular dependence of s- and p-polarized reflectivities at several wavelengths can be used in the integration of Maxwell equations to construct the spatial profile of the density of charge carriers.

Influence of optical non-uniformity on the reflectance of dense plasmas

Norman G E and Saitov I M[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] saitovilnur@gmail.com

We provide theoretical analysis of the experimental data on reflectances of shocked compressed xenon for normal incidence of laser radiation [1, 2] as well as for the dependence of s- and p-polarized reflectivity on incidence angle [3]. Three wavelengths $\lambda = 1064$ nm, 694 nm and 532 nm are considered. We use density functional theory (DFT) approach for the calculation of the dielectric function (DF) and reflectivity of the shock compressed xenon plasma. Due to the nonlocality of the applied potential, the longitudinal expression for the imaginary DF [4] is used. The real part is obtained by the Kramers-Kronig transformation. For $\lambda = 1064$ nm and 694 nm the relatively good agreement with the experiment is obtained without introduction of the wave front broadening. However, for 532 nm the calculated reflectances are overestimated in comparison with the experiment. Also the calculated Brewster angles are shifted with respect to the measured values. The discrepancy can be partially related to the nonzero width of the region with non-uniform profile of density (wave front). The width of the front is estimated [5] under assumption of the linear dependence of the DF on distance. These values are much closer to the theoretical estimate of 100 nm [1], in comparison with earlier works [2,3]. The work is supported by grant No. 14-19-01295 of the Russian Science Foundation.

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Ion recombination in dense gases

Lankin A V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

Alex198508@yandex.ru

Ion recombination is considered in a wide range of medium properties in dense gases. A dependence of the ion recombination rate on background gas density is found. Ranges of different recombination kinetics regimes are defined.

Recombination rate constant is linearly dependent on background gas density at low densities. It agrees with the Natanson model at low ion Coulomb nonideality. It is a range of collisional recombination. Its border is defined by the condition $n\sigma < L^{-1}$, where n is a neutral molecules concentration, σ is a cross-section of ion-molecule collisions, $L = e^2/kT$ is Landau length.

Langevin model is valid at high densities of the background gas. Ion recombination rate constant is inversely proportional to the background gas density. It is a range of diffusive recombination. Its border is defined by the condition $n\sigma > 4L^{-1}$. A dependence of the recombination rate on the ion Coulomb nonideality is established, contrary to the idea that there is no such dependence [1], though it is weaker than in the collisional regime. The dependence can be interpolated as exponentially drop-down curves in the whole range of the nonideality parameter values. The slope of the decay decreases with an increase of the background gas density, in other words, with the decrease of the ion free path. Extrapolation of this trend to high densities permits to suggest that the dependence is of no importance in liquids. However, the effect can be remarkable in the range of gas pressures from one up to several dozen atmospheres.

A complex nonmonotonic dependence of the recombination rate on the background gas density takes place in the intermediate region $L^{-1} < n\sigma < 4L^{-1}$. A maximum occurs in the range about $n\sigma = 4L^{-1}$. The work is supported by the RSF grant 14-19-01295.

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The movement of an electron in a molecular ion H_2^+

Vikhrev V V

National Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia

vikhrev@mail.ru

Simulation of motion of electron sitting in the field of two protons was made using Monte Carlo method.
The initial conditions were as follows: electron was on a stationary orbit with the angular momentum $h/2$ and at the nearest point to the first proton, while the second proton was on the opposite side to the first proton, at the distance $a_0 = 0.185 r_B$ (r_B—Bohr radius of the electron orbit) from the first proton. Initial velocity of electron $V_0 = h/2a_0$. The total interaction force between protons was computed taking into account the rapid movement of electron between these protons and multiple electron spin flips.
The three kind of trajectories were found for the electron:

(i) electron trajectory is similar to ellipse with both protons (approximately $2r_B$ between protons) sitting inside it, this case protons are repulsed, Coulomb force is negative,

(ii) electron trajectory is "eight-like", this case protons are attracted, Coulomb force is positive,

(iii) distance between protons are large enough, electron trajectory is elliptical, similar to case (i), but only one proton is inside this trajectory. Interaction force between protons is dramatically decreased since one of the protons becomes neutral hydrogen atom.

It was shown that the energetically profitable combintion of two protons and one electron is only possible if bonding energy is close to 2 eV.

Equation of state of a dense plasma: Analytical results on the basis of quantum pair interaction potentials in the random phase approximation

Moldabekov Zh A[@], Ramazanov T S and Gabdullin M T

Research Institute of Experimental and Theoretical Physics of the Al-Farabi Kazakh National University, al-Farabi Avenue 71, Almaty 050040, Kazakhstan

[@] zhandos@physics.kz

In the present work the analytical results for equation of state of a dense plasma was derived. The dielectric function of electrons was taken in the random phase approximation. Using expansion of the dielectric function in long wave length limit [1], pair correlation function of particles was obtained. Inner energy and contribution to the pressure due to plasma non-ideality derived for both Coulomb pair interaction and quantum pair interaction potentials [2]. Obtained analytical result for equation of state reproduces the Montroll–Ward contribution [1], which corresponds to the quantum ring sum. It was shown that obtained results cover the Thomas–Fermi approximation with the first order gradient correction. Additionally, it was revealed that the quantum Deutsch potential correct in the semi classical limit. Generalization of the quantum Deutsch potential to the case of the degenerate electrons is presented. Obtained results will be useful for understanding of the physics of dense plasmas as well as for further development of the multi-scale approach for the dense plasma simulation via molecular dynamics on the basis of the quantum potentials.

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Equation of state of dense hydrogen plasma

Ismagambetova T N[@], Gabdullin M T, Ramazanov T S, Otarbay Zh Y and Mamatova M M

Al-Farabi Kazakh National University, al-Farabi Avenue 71, Almaty 050040, Kazakhstan

[@] miriael@mail.ru

In this work effective interaction potentials taking into account quantum-mechanical effects of diffraction and symmetry were used [1, 2]. Pair correlation functions were studied in exponential approximation. Thermodynamic properties for hydrogen plasma were calculated with respect to the degree of ionization using the analytical expressions derived from these effective potentials.

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A new approach to the calculation of the Wigner function of quantum particles at finite temperature in the canonical ensemble

Larkin A S and Filinov V S[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vladimir_filinov@mail.ru

One of the most common numerical methods in quantum statistical thermodynamics is a quantum Monte Carlo method based on the representation of physical quantities in the form of a path integrals (Wiener and Feynman integrals). Another approach is based on the use of quantum Wigner function in the phase space, which in many ways is similar to the distribution in the classical statistical physics and is in fact a real representation the density matrix. In addition, the Wigner formalism opens the way to the calculation of transport properties.

We present a new approach to calculation of the Wigner function of quantum particle system at finite temperature in the canonical ensemble, for which it is developed a new form of a path integral. The new Monet Carlo method enables to calculate the thermodynamic values, the Wigner function itself and even the ground-state wave functions. The developed formalism has been tested and demonstrated good accuracy of these calculations. In addition, the developed method allows to calculate the thermodynamic averages of arbitrary operators, which can not be done by conventional methods. Preliminary calculations of many-particle Wigner function for the non-ideal hydrogen plasma have been carried out.

The thermophysical properties of Fe plasma

Apfelbaum E M

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

apfel_e@mail.ru

The thermophysical properties (equations of state and electronic transport coefficients) play important role both in theory and applications. They have been calculated and measured for dozen years. Now we have several theoretical approaches to obtain the necessary information in the metallic plasma region (see [1] for references). But at relatively high temperatures ($T \geq 5$ kK), where the plasma of metals is located, the number of measurements is significantly smaller than the number of calculations. Besides the temperature can not be measured directly in the experiments yet. Nevertheless, the available measurement data [2–5] allows one to check the existing calculation models.

Earlier we have developed the model to calculate the chemical composition, thermodynamical values and electronic transport coefficients for the plasma under study. It was applied to noble gases, several metals and semiconductors (see references in [6]). It is based on the "chemical" approach (to find the plasma composition and thermodynamical values) and the relaxation time approximation (to find the coefficients). Here our model has been applied to study Iron plasma properties, namely the pressure, internal energy, conductivity, thermal conductivity and thermal power at $T \geq 10$ kK and $\rho \leq 2$ g/cc. The obtained results are in good agreement with available results of measurements and calculations of other authors.

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Dynamical equations and transport coefficients for the metals at high pulse electromagnetic fields

Volkov N B[1,@], Chingina E A[1] and Yalovets A P[2]

[1] Institute of Electrophysics of the Ural Branch of the Russian Academy of Sciences, Amundsen 106, Ekaterinburg 620016, Russia
[2] South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia

[@] nbv@iep.uran.ru

The aim of our work is construction of metal model, suitable for the description of high-speed electrophysical processes in pulse strong electromagnetic fields. It is necessary, that metal represents a mix of two "liquids": the ionic, consisting ion skeletons of identical weight occupying sites of a deformable lattice, and electronic, containing electrons of a continuous spectrum. Also in our model the electron transitions between localized (discrete) and delocalized (continuous) states with total rate $\Gamma_e = \delta n_e/\delta t$ are taken into account. With the help of the approach proposed by Andreev and Pushkarov [1] we deduced the two-liquid, two-temperature equations for describing of metal interaction with a pulse electromagnetic field within the framework of full Maxwell equations system in view of generation and recombination of the conduction electrons, and their inertia.
With the help of known methods the kinetic equations for phonons and conduction electrons in a deformable crystal lattice are solved, and expressions for electron and phonon transport coefficients in pulse high electromagnetic fields are deduced. It is shown, that the electronic transport practically does not depend on intensity of an electromagnetic field until degeneration of the conduction electrons is removed.
The work carried out within the state order No. 0389-2014-0006 and under the partial financial support of the RFBR (project No. 16-08-00466) and the Ural Branch of RAS within the UB RAS fundamental research program "Matter at high energy densities" (project No. 15-1-2-8).

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Reflecting boundary conditions for classical molecular dynamics simulations of nonideal plasmas

Lavrinenko Ya S[1,2,@], Morozov I V[1,2] and Valuev I A[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] lavrinenko@phystech.edu

Theoretical studies of strongly coupled systems of charged particles such as electron-ion nonideal plasmas, ion liquids, dusty plasmas, etc. often rely on atomistic simulations by the methods of classical Molecular Dynamic (MD) and Monte-Carlo (MC). For both methods there is a long standing boundary condition problem when modelling an infinite spatially uniform system of particles interacting via the long-ranged Coulomb forces. The influence of boundary conditions for the classical molecular dynamics (MD) simulations of nonideal electron-ion plasma is studied in this work.
We start with the classical MD and perform a comprehensive study of convergence of the per-particle potential energy and pressure with the number of particles using both thenearest image method (periodic boundaries) and harmonic reflective boundaries. It allows one to estimate an error caused by finiteness of the simulation box. Moreover electron oscillations given by the spectra of the current autocorrelation function are analysed for both types of the boundary conditions. A special attention is paid to the reflecting boundaries since they prevent wave packet spreading in the Wave Packet MD. To speedup classical MD simulations we use the GPU-accelerated code.
This work is supported by the Russian Science Foundation, grant No. 14-19-01295

Relativistic free matter expansion

Ignatov A M[1,@] and Trigger S A[2]

[1] Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova 38, Moscow 119991, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] aign@fpl.gpi.ru

The relativistic hydrodynamic expansion of free matter is considered to describe some specific pecuiliartities of the cosmological model of the gravitationally neutral Universe—GNU-Ball [1, 2]. On this basis the Hubble flow hydrodynamic solution for the non-relativistic case [3] is generalized for the relativisic dynamics. Starting from equations

$$\frac{\partial n(t,\mathbf{r})}{\partial t} + \nabla(n(t,\mathbf{r})\mathbf{V}(t,\mathbf{r})) = 0, \tag{1}$$

$$\frac{\partial \mathbf{P}(t,\mathbf{r})}{\partial t} + \mathbf{V}(t,\mathbf{r})\nabla(\mathbf{P}(t,\mathbf{r}) = 0, \tag{2}$$

where

$$\frac{\partial \mathbf{P}(t,\mathbf{r})}{\partial t} + \mathbf{V}(t,\mathbf{r}) = \frac{c\mathbf{P}(t,\mathbf{r})}{\sqrt{P^2(t,\mathbf{r}) + m^2c^2}}, \tag{3}$$

we arrive at equation for velocity

$$\gamma^3(\mathbf{V}(t,\mathbf{r}))\frac{\partial \mathbf{V}(t,\mathbf{r})}{\partial t} + \mathbf{V}(t,\mathbf{r})\nabla(\mathbf{V}(t,\mathbf{r}) = 0. \tag{4}$$

Here $\gamma = 1/\sqrt{1 - V^2/c^2}$. This mens that the solution is identical to [3] if $V(t,\mathbf{r}) < c$. Over this horizon hydrodynamics does not applicable.

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Degenerate Bose gas without anomalous averages

Bobrov V B[@] and Trigger S A

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vic5907@mail.ru

Theory of a weakly non-ideal Bose gas in the canonical ensemble is developed without assumption of the C-number representation of the creation and annihilation operators with zero momentum. Instead of this assumption, we use the assumption on the C-number nature of the density operator $N_0 = a_0^\dagger a_0$ with zero momentum. It is shown that the pole of the "density-density" Green function (DDGF), and the pole of the single-particle Green function (SPGF), exactly coincide with the Bogoliubov phonon-roton spectrum of excitations for both assumptions. This spectrum, confirmed by many neutron and X-ray experimental measurements of the dynamic structure factor in HeII, is straightly related to the DDGF. We show that in the other case under consideration, when neither N_0 nor $a_0^\dagger$ and a_0 are C-numbers, a gap can exist in the single-particle Green function (SPGF). This gap in SPGF excitations is straightly related to the density of particles in the "condensate". Therefore, the spectra of excitations for the DDGF and SPGF in the last case are different [1], in contrast to the Bogoliubov-type theory where these spectra are identical. We arrive at the conclusion that there are two various versions of the weakly non-ideal Bose gas theory with different pole structures in DDGF and SPGF. The choice between these two versions should be made in indirect way based on the calculations of the thermodynamic functions of HeII and ultracold rarified gases, and the comparison of these calculations with experiments in a wide temperature range, including the vicinity of the superfluid-to-normal state transition temperature in HeII.

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Thermionic emission from nanoplasma

Bystryi R G[1,2,@] and Morozov I V[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] National Research University Higher School of Economics, Bolshoy Tryokhsvyatitelsky Pereulok 3, Moscow 123022, Russia

[@] broman.meld@gmail.com

The nanoplasma produced by laser pulses of moderate intensities (10^{13}–10^{16} W/cm^2) targeted at metal clusters is studied by molecular dynamics (MD) simulations. Whereas a lot of the cluster plasma studies are concerned with the Coulomb explosion of the ion core we focus on the electron dynamics just after cluster ionization. In particular we consider electron eigenmodes and electron emission depending on the cluster size and plasma temperature.

One of the distinguishing features of the cluster plasma is the violation of the plasma neutrality [1]. Due to the laser ionization and further thermionic emission from the plasma surface the cluster gains an uncompensated positive charge. With respect to a small number of particles in the clusters under consideration (10–10^6) this charge determines the rate of plasma expansions, affects the rate of ionization-recombination processes, electron density profile, and optical properties of the cluster plasma [1, 2].

In this work we propose a model of thermionic emission of nanoclusters based on our MD simulation results [3]. This model qualitatively explains known experimental results [4] and it is in a good agreement with other simulations [5].

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Current–pressure dependencies of dc magnetron discharge in inert gases

Serov A O[1,2], Mankelevich Yu A[2,1], Pal A F[1,2] and Ryabinkin A N[1,2,@]

[1] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 142190, Russia

[2] Skobeltsyn Institute for Nuclear Physics of the Lomonosov Moscow State University, Leninskiye Gory 1, Moscow 119899, Russia

[@] alex.ryabinkin@gmail.com

The dependence of current–pressure (I-P) characteristics of dc magnetron discharge at a constant voltage on the type of working gas was investigated. Under certain conditions on the I-P characteristic the nonmonotonic region of local maximum followed by a minimum is observed. It is found that increasing mass of the working gas ions results in a shift of the local maximum to lower pressures. The spacial distributions of ions in the plasma on different discharge conditions were studied with optical emission spectroscopy. A qualitative model of the phenomena is presented and its results are compared with the experimental data.

The work was supported by the Russian Foundation for Basic Research, grant No. 15-02-06873.

Streamer branching on clusters of solid particles in air and air bubbles in liquids

Babaeva N Y[@], Tereshonok D V, Naidis G V and Smirnov B M

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] nybabaeva@gmail.com

Streamer branching—the splitting of a discharge filament into two or more streamers—is a common phenomenon that occurs in high pressure gases and liquids. The evolution of the streamer depends on its local environment and the presence of inhomogeneities in the path of a streamer. In this work, we present the results from a two-dimensional computational investigation of the intersection of a streamer with clusters of particles or gas bubbles. We consider the evolution of a streamer propagating along the vector of the electric field (which is directed vertically). The clusters of particles in air or bubbles in liquids have a symmetric form with branches elongated either in horizontal or vertical direction. In gases, the streamer envelopes the particles while in liquids the discharge preferably occurs inside the bubbles. The orientation of the cluster determines the branching pattern. We show that clusters having prevailing horizontal branches facilitate streamer branching in liquids, while clusters in gases with vertical branches promote the splitting of a discharge filament into two or more streamers. The phenomenon is mainly due to different polarization patterns of "vertical" or "horizontal" clusters and the resulting ratio of dielectric permittivity of medium/particle or medium/bubble. We consider two opposite cases (i) when the dielectric permittivity of the medium is unity (air) and the dielectric permittivity of particles ranges from 1 to 80 and (ii) the case when the dielectric permittivity of bubbles (filled with air) is unity and the dielectric permittivity of medium (liquids) varies from 1 to 80. This work is supported by the Russian Science Foundation (Project Number 14-50-00124).

Investigation of synthetic jet magnetohydrodynamic actuator

Kazanskiy P N[@], Moralev I A, Efimov A V, Firsov A A and Karmatskiy R E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] fokkoo@yandex.ru

Current paper presents study of previous work [1]. It has been revealed that an arc discharge ignition ($I = 300$ A) in a magnetic field ($B = 0.2$ T) inside the channel leads to the formation of an induced jet. The research was performed for the $2 \times 5 \times 80$ mm^3 test chamber. The dynamic flow visualization of the jet after a single discharge ignition was performed. Mean discharge power was no more than 200 W. Evolution of the flow after a single magnetohydrodynamic (MHD) actuator pulse was investigated experimentally by Schlieren photography and particle image velocimetry. The Schlieren photography shows that the pulse energy input causes a compression wave. It has been found that the maximum velocity of thermal point was more than 200 m/s. The velocity of thermal point decreases up to 80 m/s after 0.160 ms. At the same time the leading edge of the thermal point moves at 16–23 mm from the nozzle. In other hand the flow velocity inside the jet in a predetermined configuration may be up to 540 m/s. The actuator was mounted as a pendulum for the pulse measurement. The maximum pulse of the induced jet by single discharge ignition was 10^{-4} kg m/s. The MHD synthetic jet generator efficiency is higher than thermal and dielectric-barrier-discharge synthetic jet generator. Current method can be useful for flow control on a par with mechanic synthetic jet generator.

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Active flow control on a NACA 23012 airfoil model by means of magneto-hydrodynamic plasma actuator

Kazanskiy P N[@], Moralev I A, Bityurin V A and Efimov A V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] fokkoo@yandex.ru

The paper presents investigation of previous work [1]. It has been revealed that an arc discharge ignition in a magnetic field of plasma actuator leads to change main airfoil aerodynamic coefficients C_x, C_y and longitudinal moment. The research was performed for the NACA 23012 airfoil model at flow velocities of up to 60 m/s (134 mph). The dynamic flow visualization of an airfoil model after a single discharge ignition was performed. Mean C_y change and the longitudinal moment M change were no more than 5% at pulse repetition frequency 13 Hz. The amplitude of lift change was not more than 10%, the amplitude of longitudinal moment change was not more than 5%. Time resolution of strain scales was more than 30 ms. It was not possible to resolve the real change of lift force during the discharge pulse. The amplitude was significantly reduced (approximately by 20–50 times). Mean discharge power was no more than 200 W. The magneto-hydrodynamic (MHD) actuator was mounted on the upper side of the wing model. Evolution of the flow after a single MHD actuator pulse was investigated experimentally by particle image velocimetry. It has been found that the velocity of the arc in a predetermined configuration may be up to 250 m/s. The upstream movement of the arc channel (I = 40–700 A) leads to the inhibition and high pressure zones before the arc and local low pressure cavity.

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Flow around circular cylinder induced by arc discharge rotating in magnetic field

Munhoz D S[@], Klimov A I, Bityurin V A and Moralev I A

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] dasmunhoz@yahoo.com.br

The field of plasma aerodynamics is intensively being developed worldwide. The emphasis of these works was focused on the study of the flow control around aerodynamic models with the use of local plasma formation on the surface of the model [1–5]. An experimental study of the airflow around a circular cylinder was fulfilled on subsonic regime. The flow was subjected to a rotating arc discharge around the cylinder model due to external radial magnetic field. Measurement of aerodynamic forces of the cylinder model, after turning on the arc discharge, showed immediate lift force response and air circulation around its surface, induced by the moving arc discharge.

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Experimental and theoretical study of the microwaves transmission through plasma structures and layers in a constant magnetic field

Bocharov A N[1], Bityurin V A[1], Brovkin V G[1], Vedenin P V[1], Petrovskiy V P[1,@], Balakirev B A[2], Korneev V N[2], Pashchina A S[1] and Shkatov O Yu[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Open Joint Stock Company "Corporation Moscow Institute of Heat Technology", Beryozovaya Avenue 10, Moscow 127273, Russia

[@] b1p2a3@mail.ru

The possibility of significant improvement transmission conditions of microwave radiation passing through a homogeneous quasi-neutral plasma layer in the constant magnetic field is considered The study based on 1D analysis was conducted for layers with electron concentration 10^{17}–10^{19} m^{-3} and collision frequency of electrons with molecules 10^{10}–10^{11} s^{-1} in the wavelength range 1–10 cm. For different values of plasma parameters the dependences of the magnetic induction values were obtained reducing a transmitted wave amplitude attenuation to a specified level (3 dB). The influence of the angle between vectors B_0 and k on the wave amplitude revealed the optimal conditions of the field B_0 orientation relative to the direction of electromagnetic waves propagation. the influence of a constant magnetic field on the attenuation degree of microwave radiation ($f = 13$ GHz) in a various types plasma structures and in the plasma layers was experimentally investigated. The experiments were carried out in air at pressures 70–500 Torr. A remarkable increase in the amplitude of the transmitted wave in presence of constant magnetic field was indicated.

Magneto-plasma compressor for radiophysical study of supersonic flows around bodies

Bocharov A N[1], Bityurin V A[1], Brovkin V G[1,@], Mashek I Ch[1], Vedenin P V[1], Balakirev B A[2], Petrovskiy V P[1], Pervov A Yu[2] and Shkatov O Yu[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[2] Open Joint Stock Company "Corporation Moscow Institute of Heat Technology", Beryozovaya Avenue 10, Moscow 127273, Russia

[@] brovkin47@mail.ru

One of the promising applications of Magneto-Plasma Compressor (MPC) may be using plasma jets generated by MPC for experimental study of hypersonic flow around the models. For the study the MPC was developed with a caliber of 24 mm with internal initiation of discharge, working in "submerged" mode. The maximum operating value of the discharge current in this MPC corresponds 29 KA, the duration of the current pulse is not less than 90 microseconds. Jet quazi-stationary mode is set when the discharge current reaches of about 12–15 KA, that gives an estimate of the jet lifetime about 55–60 μs. To estimate the abilities of MPC the tests were conducted with Teflon conic models with a diameter of 10 mm and a height of 30 mm at a distance from the edge of the cone to the MPC nozzle exit 30–50 mm. Experiments have shown that the studied type of the MPC could serve as a basis for creation of the experimental stand for the radio physical researches of the processes in hypersonic flows in the ranges of pressures and flow rates of interest.

Approach to solution of coupled heat transfer problem on the surface of hypersonic vehicle of arbitrary shape

Bocharov A N[1,@], Bityurin V A[1], Golovin N N[2], Evstigneev N M[1], Petrovskiy V P[1], Ryabkov O I[1], Teplyakov I O[1], Shustov A A[2], Fortov V E[1] and Solomonov Yu S[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Open Joint Stock Company "Corporation Moscow Institute of Heat Technology", Beryozovaya Avenue 10, Moscow 127273, Russia

[@] bocharov@ihed.ras.ru

In this paper an approach to solve coupled heat- and mass-transfer problems is considered to be applied to hypersonic vehicle surface of arbitrary shape. The approach under developing should satisfy the following demands. (i) The surface of the body of interest may have arbitrary geometrical shape. (ii) The shape of the body can change during calculation. (iii) The flight characteristics may vary in a wide range, specifically flight altitude, free-stream Mach number, angle-of-attack, etc. (iv) The approach should be realized with using the high-performance-computing (HPC) technologies. The approach is based on coupled solution of 3D unsteady hypersonic flow equations and 3D unsteady heat conductance problem for the thick wall. Iterative process is applied to account for ablation of wall material and, consequently, mass injection form the surface and changes in the surface shape. While iterations, unstructured computational grids both in the flow region and within the wall interior are adapted to the current geometry and flow conditions. The flow computations are done on HPC platform and are most time-consuming part of the whole problem, while heat conductance problem can be solved on many kinds of computers.

Gasliquid type phase transition in modified pseudopotential and "shelf Coulomb" ultracold plasma models

Butlitsky M A[@], Zelener B B and Zelener B V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] aristofun@yandex.ru

Phase diagrams for both "shelf Coulomb" and modified pseudopotential plasma models, developed in our previous works are compared. Qualitative agreement is observed between gas–liquid phase transition region of "shelf Coulomb" model and liquid—gas structure region of modified pseudopotential one. The possibility of experimental finding the phase transition in nonequilibrium ultracold rydberg plasma is considered. Parameters (density, temperature, levels of rydberg atoms) for such a transition are estimated.
Conclusion is made that "shelf Coulomb" model phase transition is practically impossible to observe in equillibrium strongly coupled plasmas due to high neutral atoms density at low temperatures: $T^*_{\text{crit}} \approx 0.076$. The work is supported by Russian Science Foundation (RNF14-50-00124 grant).

On the temperature of antihydrogen formed in magnetic trap

Bobrov A A[@], Bronin S Y, Manykin E A, Zelener B B, Zelener B V and Khikhlukha D R

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] abobrov@inbox.ru

In the experiments in CERN antihydrogen is formed during mixing of antiprotons and positrons in Penning-Malmberg trap. Positrons and antiprotons form nonneutral plasma with $n_e = 10^8 cm^{-3}$ and $n_p = 10^4 cm^{-3}$. Initial energies of antiprotons and temperatures of positrons are varied in wide range: $15 - 50$ K for positrons and $1 - 150000$ K for antiprotons. During mixing, energy of antiproton changes and after recombination formed atom of antihydrogen has energy of heavy particle–antiproton. It is important to know the value of this energy to effectively capture antiatoms. In this work we performed calculations of energy relaxation processes and made estimations of final antiproton energy in the moment of recombination of the antiproton and positron in strong magnetic field depending on the initial energies of antiprotons and positrons. It was shown that for some initial conditions antiproton energy may reach the positrons temperature and for some conditions the recombination time is less than relaxation time. Moreover relaxation rate for axial and transverse to magnetic field antiproton velocity components is different.

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Dipole–dipole interaction between Rydberg atoms

Zelener B V[@], Bronin S Y, Dyachkov L G and Klyarfeld A B

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] zelener@ihed.ras.ru

The applicability of van-der-Waals potential approximation (C_6/R^6) is limited by its smallness in comparison with the distance to the nearest undisturbed level of the system of two interacting atoms. It is shown that this condition should be taken into account in the interaction of Rydberg atoms. The calculation of the interaction potential for one of Δ-term system of two ^{7}Li atoms in the 5d state is given. It is shown that the violation of the specified conditions, the dependence of the potential $1/R^6$ is replaced by the linear dipole interaction dependence $1/R^3$, resulting from the solution of the secular equation.

The work was supported by grants of the RFBR 14-19-01492.

Study of Rydberg states of the lithium atoms

Zelener B B[@], Saakyan S A, Sautenkov V A, Zelener B V and Fortov V E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] bobozel@mail.ru

We will present a new experimental result of precise measurements of forbidden and allowed Rydberg state's ^{7}Li energy. We have studied of highly-excited states of ultracold lithium-7 atoms by using tunable uv-laser. The diagnostic of Rydberg transitions of lithium atoms in magneto-optical trap is developed [2]. In our work the results for different Rydberg states ns, np, nd, nf with quantum number n from 38 to 161 will be presented. The work was supported by the Russian Science Foundation, project No. 14-12-01279.

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Coherent and non-coherent components of two-step excitation in Rydberg states of ultracold lithium media

Vilshanskaya E V[1,2,@], Saakyan S A[1], Sautenkov V A[1,3] and Zelener B B[1,4]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia
[3] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia
[4] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

[@] eva.villi@gmail.com

Energy spectra of ultracold Rydberg lithium atoms are discussed. Our technique [2] has been used for the experimental observation coherent and non-coherent components of two-step excitation in Rydberg states. The high sensitivity of the technique has allowed us to record coherent resonance 2P-38D. The width this resonance is 3 times less than non-coherent. The coherent resonance is observed when the laser is detuned by $\pm$ 803.5 MHz from the atomic transition $2P_{3/2}$.

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Measurments of ionization energy for lithium-7

Saakyan S A[@], Sautenkov V A, Zelener B B and Zelener B V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] saasear@gmail.com

The goal of this work is the experimental study of the ionization energy of the lithium atom 7. For the detection of highly excited states of lithium 7 we used the resonance fluorescence registration technique [1]. The ionization energy was calculated by using our experimental data [2]:

$$E_i = 43487.15739(39)\ \mathrm{cm}^{-1}.$$

Standard experimental methods are used diagnostics based on ionization by an electric field [3]. In this work we used the technique based on recording of resonance fluorescence of the trapped atoms. It is important that our measurements do not destroy the Rydberg states of ultracold atoms. Measured value are in good agreement with theoretical results [4,5]. Due to a weak residual field the energy levels were shifted by quadratic Stark effect. Using our measured energy values we estimated the residual field as 10^{-2} V/cm [2].
The work was supported by the Russian Science Foundation, project No. 14-50-00124.

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Measurements of quantum defect in Rydberg d-states for lithium atoms

Murashkin D A[1,2,@], Saakyan S A[1], Sautenkov V A[1,3] and Zelener B B[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[3] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

[@] 3995@mail.ru

We have developed an effective spectroscopic method for diagnostic of highly excited ultracold atoms using the registration of resonance fluorescence of atoms in magneto-optical trap during two-step cw excitation of Rydberg states by uv laser [1]. The value of the quantum defect was determined for Rydberg states nd of lithium-7 atoms $\delta = 0.00192(17)$.

The work was supported by Research Center FAIR (FAIR, Russia), MK-4092.2014.2, NSh-6614.2014.2, the RFBR 14-02-00828, the Presidium RAS (basic research program "Investigation of Matter in Extreme States" headed by V E Fortov).

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Calculations of rf plasma flow with metastable atoms at low pressure

Shemakhin A Yu[1,@] **and Zheltukhin V S**[2]

[1] Kazan Federal University, Kremlyovskaya 18, Kazan, Tatarstan 420008, Russia

[2] Kazan National Research Technological University, Karl Marx Street 68, Kazan, Tatarstan 420015, Russia

[@] shemakhin@gmail.com

Plasma rf discharges at low pressure (13.3–133 Pa) with gas blowing is effectively used to modify the surfaces of materials of organic and inorganic nature [1]. The plasma, which created by discharge of this type has the following properties: degree of ionization of 10^{-4}–10^{-7}, electron concentration 10^{15}–10^{19} m^{-3}, the electron temperature is 1–4 eV, the temperature of atoms and ions is 3–4 kK in the bunch and 0.32–1 kK in the plasma jet. Flow of neutral component is in a transitional mode between the continuum mode and free-molecule flow, the charged components can be approximated of continuous medium [2]. The concentration of metastable atoms for this type of plasma can reach values of the electron density.

Mathematical model of rf plasma flow at low pressure with metastable atoms influence is constructed. Calculations of the undisturbed flow of rf plasma at low pressure are completed. The distributions of the velocity modulus, pressure and temperature of the carrier gas and the electron concentration, electron temperature are obtained.

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Structure of the metal films deposited on small spheres trapped in the rf magnetron plasma

Filippov A V[1], Pal A F[1,2], Ryabinkin A N[1,2] and Serov A O[1,2,@]

[1] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 142190, Russia
[2] Skobeltsyn Institute for Nuclear Physics of the Lomonosov Moscow State University, Leninskiye Gory 1, Moscow 119899, Russia

[@] aserov@mics.msu.su

The metallic coatings were deposited onto the glass spheres having diameters from few to one hundred micrometers by the magnetron sputtering. Two different experimental schemes were used. One of them was the traditional configuration where the magnetron sputter was placed at 10 cm from the particles. Continuous mechanical agitation in the fluidized bed was used to achieve uniformity of the coatings in the case. In the second scheme the treated particles levitated in the magnetron rf plasma over the sputtered target (rf electrode) at the small distance d of few mm from it and at relatively high gas pressure p up to 100 mTorr, which were quite different from ones in the traditional sputtering. Agitation due the features of particles confinement in the dusty plasma was used here to obtain uniform coatings. It was observed that in the case of magnetron rf dusty plasma the product pd value may be achieved which is several times lower than the lowest value proper to the first, traditional case. The thickness and morphology of the obtained coatings were studied. The dependencies of the films growth rate and structure on the pd value in these sputtering processes are quite different. The dependencies are qualitatively described basing on consideration of the links between the product value and the actual parameters such as the substrate temperature, the densities of the ion and neutral atom fluxes to the substrate surface.
The work was supported by the Russian Foundation for Basic Research grant No. 15-02-06873.

Interaction in equilibrium plasmas of charged macroparticles located in nodes of cubic lattices

Filippov A V

State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 142190, Russia

fav@triniti.ru

Interaction of two charged pointlike macroparticles located at nodes of simple cubic (sc), body-centered cubic (bcc) and face-centered cubic (fcc) lattices in equilibrium plasma is studied within the Debye–Hückel approximation, i.e., based on the linearized Poisson–Boltzmann model. A method of solution this problem with outer boundaries of complex shapes is outlined in [1] (see also [2]). It is shown that the boundary shape has a strong influence on the electrostatic interaction between two macroparticles, which switches from repulsion at small interparticle distances to attraction as it approaches the half-length of the computational cell. It is found that in the case of dust particles arranged in the nodes of the sc, bcc and fcc lattices, the electrostatic force acting on them is equal to zero and the nature of the interaction changes from repulsion to attraction; hence, infinite sc, bcc and fcc lattices of charged dust particles are mechanically stable.

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Dynamics and ordering in small systems of interacting particles

Koss X G[@], Petrov O F, Myasnikov M I, Statsenko K B and Vasiliev M M

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] Xeniya.Koss@gmail.com

We use the concept of the "dynamic entropy" [1–3] in its simple approach called "mean first-passage time" (MFPT) dynamic entropy [4] to study numerically and experimentally obtained small systems of interacting particles.

The experiments were carried out in the quasi-two-dimensional system of 7 dust grains in gas discharge plasma. This system was also simulated with the help of Langevin molecular dynamics method. The interparticle interaction potential was taken to be of Yukawa type; for the details see [5].

We have obtained the MFPT entropy functions for the systems under study and analyzed them to find out their phase states. The character of motion for different states was examined using the functions of dependence of mean-square displacement of particles on time.

The suggested technique of the analysis of the system dynamics can be applied to the structures as small as desired, independent on the degree of the thermal isolation of the system.

This work was supported by the Russian Science Foundation (project No. 14-12-01440).

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Dusty plasma as unique object of collisional plasma physics

Norman G E and Timofeev A V[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] mail.timofeev.av@gmail.com

The basic openness and self-consistency of dusty plasma system, the particle charge inconstancy in time, charge dependence on the environment parameters, high dissipation, significant influence of stochastic processes and self-organization lead to the appearance of a number of unusual properties and phenomena that occur only in dusty plasmas. Precisely this meaning is put into the term of uniqueness of dusty plasmas. The beginning of this area is put in [Norman G E, Stegailov V V and Timofeev A V 2011 *JETP*, Norman G E and Timofeev A V 2011 *Phys. Rev. E*], which are first to formulate the equation of dust particles motion with account of dust particles charge fluctuations, the dependence of the charge on the position in near-electrode layer and the proximity of other dust particles, gas discharge sheath features. Here we discuss the mechanisms and consequences of the following phenomena.
(i) *"Anomalous heating" and energy transfer in dusty plasma system.* The dust particles average kinetic energy may exceed the value of electron temperature and can be as high as thousands of eV.
(ii) *Anisotropy of the temperature and plasma properties.* The average kinetic energy of the vertical motion may differ significantly from that of horizontal motion, but each of them has a normal distribution and may be considered as in partial equilibrium.
(iii) *Dust particle charge fluctuations.* Significant charge fluctuations alter the interparticle interaction potential, make stochastic component significant and lead to a set of unique effects.
(iv) *The interparticle interaction potential.* Unique properties of the interaction potential of dust subsystem (self-consistency, many-particle, fluctuation, anisotropy) has a direct impact on the "anomalous heating", which hung up the chain of the research.
This work is supported by the RSCF (project No. 14-19-01295).

Energy transfer between degrees of freedom of a dusty plasma system

Semyonov V P[1,2,@] and Timofeev A V[2]

[1] Moscow Institute of Electronics and Mathematics, National Research University Higher School of Economics, Tallinskaya 34, Moscow 123458, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] VPSemenov@gmail.com

Phenomenon and mechanisms of an energy transfer between degrees of freedom of a dusty plasma system are of great interest in the field of dusty plasma. One of such mechanisms is based on parametric resonance [1]. Initial stages of such phenomena can be described by the equation close to Mathieu equation [1, 2]. Approach shown in [2] works only when amplitudes of particles oscillations are much smaller than interparticle distance and can not describe saturation stage.

Model of dusty plasma system including fluctuations of dust particles charge and features of near-electrode layer is used.

Using numerical approach conditions of beginning of energy transfer between degrees of freedom, growth rates of energy and saturation energy of fluctuations are obtained for a wide range of parameters. Dependence on such parameters as friction coefficient, normalized vertical gradient electric field component in the near-electrode layer, normalized vertical gradient of the dust particle charge, caused by changes in the concentrations of electrons and ions in the electrode layer and normalized amplitude of stochastic charge fluctuations, caused by fluctuations and discreteness of ions and electrons flow on the surface of dust particles is shown.

Obtained results are compared with experimantal data and allow to describe energy transfer in dusty plasma more accurate.

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Screening length in dusty plasma crystals

Nikolaev V S[1,2,@] and Timofeev A V[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] vladiorussia@mail.ru

Particles interaction and value of the screening length in dusty plasma still are of great interest in dusty plasma area. In this work three potential models (Debye potential [1], Gurevich potential [1] as simple ones and a more difficult potential coming from the Poisson's equation in both collisionless and non-collisionless modes [2]) are used to describe dusty particles interaction in order to get the theoretical dependence of interparticle distance on temperature and pressure of the neutral component. The value of the screening length in dusty plasma at different temperatures is counted from the experimental data analysis. The results are compared with experimental data by R Kh Amirov, I S Samoylov and V P Baev [3] and S N Antipov [4] studied plasma in a vertical tube in dc glow discharge. The counted value of the screening length is approximately 50 times larger than the Debye length in plasma. We thank R Kh Amirov, I S Samoylov, V P Baev for providing the results of the experiment. This work is supported by the Russian Science Foundation (project No. 14-19-01295).

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Problem of phase transitions and thermodynamic stability in complex (dusty, colloid etc) plasmas

Martynova I A[1,2,@] **and Iosilevskiy I L**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] martina1204@yandex.ru

Features of the first-order phase transitions in complex (dusty, colloid etc.) plasma are under discussion. The base for consideration is the well-known phase diagram of dusty plasma as an equilibrium Debye system [1] in Γ–κ plane (Γ is a Coulomb non-ideality parameter, κ is a screening parameter). The initial Γ–κ phase diagram [1] is converted in standard thermodynamic variables in temperature–pressure–density planes. The melting density gap in Yukawa system was estimated based on the hypothesis of similarity for melting properties of repulsive Yukawa and Soft Spheres systems. Extensive area for *negative compressibility* of the system was revealed at phase diagramin a fluid state of initial Debye system when one considers the system as equilibrium two-component electroneutral mixture of macro- and microions ($+Z$,-1) under equations of state [1] and [2]. This means *thermodynamic instability* of simplified Debye system in this domain. Non-linear screening and unavoidable existence of additional phase transitions of gas–liquid and gas-crystal type are proposed as hypothetical resolution of discussed thermodynamic instability problem.

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International research laboratory and planned hydrodynamic experiments at the International Space Station

Son E E[1,@], Fortov V E[1], Gorshkov O A[2], Zelenyi L M[3], Kabov O A[4], Karabadjak G F[2] and Tsurkov V I[5]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Central Scientific Research Institute of Machine Building, Pionerskaya Street 4, Korolev, Moscow Region 141070, Russia
[3] Space Research Institute of the Russian Academy of Sciences, Profsoyuznaya 84/32, Moscow 117997, Russia
[4] Institute of Thermophysics of the Siberian Branch of the Russian Academy of Sciences, Academician Lavrentyev Avenue 1, Novosibirsk-90 630090, Russia
[5] Dorodnitsyn Computing Center of the Russian Academy of Sciences, Vavilova 40, Moscow 119333, Russia

[@] son.eduard@gmail.com

Currently, the International Space Station (ISS) has 4 research modules (of Russia, the United States, Europe and Japan) for leading scientific experiments. Later on the modules is expected to create research laboratories with modern equipment. Some of these laboratories already exist and new ones to be created. These include cold atom laboratory (CAL), fluid dynamics, combustion, plasma, biology, medicine and others. This report discusses the new Russian proposals for the ISS, and the participation of Russian research groups in the field of hydrodynamic experiments. It proposed to conduct experiments on the dynamics of Bose–Einstein condensation, where in microgravity do not need to build complex configuration traps compensated gravity field in the laboratory of cold atoms. In the laboratory on combustion, proposed experiments are on turbulent combustion mixed and unmixed mixture of fuel and oxidizer, which can provide answers to the fundamental questions of the theory of turbulent combustion in terrestrial conditions. The aim of the report is to draw the attention of specialists to the formulation of the new tasks for the ISS in established research laboratories.

The cosmic dust: Dynamic and interaction with solar system objects

Dolnikov G G[1,@], Zakharov A V[1], Kuznetsov I A[1], Lyash A N[1], Popel S I[1], Kopnin S I[1], Shashkova I A[1], Izvekova Yu N[1], Morozova T I[1] and Rozenfeld E V[2]

[1] Space Research Institute of the Russian Academy of Sciences, Profsoyuznaya 84/32, Moscow 117997, Russia
[2] Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, Sofya Kovalevskaya Street 18, Ekaterinburg 620219, Russia

[@] ggd@iki.rssi.ru

Cosmic dust particles what played a major role in the formation of the solar system, continue to have a significant effect on the majority of cosmic objects on the present stage of its evolution. Processes related with solid particles from 1 mm till nano-sized, contribute to the formation of surfaces, atmospheres and exospheres many celestial bodies, ranging from asteroids and comets, and ending with the planetary system as a whole. The dust processes are responsible for the formation of the external surface and the planet's climate, for example, in the case of Mars, productions of the levitating dust phenomenon near the surface none atmospheric bodies Moon, Phobos, Mercury, asteroids, eruptions of the dust particles and aerosols contained in the ice and the liquid phase substance Enceladus, comets, the presence of the rings and tors (of Saturn, Jupiter, etc.). These phenomena are very interesting and can to supplement our knowledge about specific physical mechanisms of the involvement of the dust component in the observed dynamic processes. The set of the numerous theoretical models describing the dynamics of dust particles, often contradict each other and observations, and should be clarified and/or experimentally confirmed. This work is present the estimations of theoretical and experimental development of methods of modeling of processes of formation and dynamics of dust and dusty plasma phenomena surrounding the cosmic bodies of the Solar system. Usage numerical methods for an experimental setup will allow developing and improving existing methods of registration of dust particles and electrostatic fields influencing on their dynamics.

Effect of an electric field on a Coulomb cluster confined in a cusp magnetic trap under microgravity conditions

Dyachkov L G[1,@], Myasnikov M I[1], Petrov O F[1], Vasiliev M M[1], Fortov V E[1], Savin S F[2] and Serova E O[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Korolev Rocket-Space Corporation "Energia", Lenin Street 4a, Korolev, Moscow Region 141070, Russia

[@] dyachk@mail.ru

On the board of the International Space Station, in the framework of the experiment "Coulomb Crystal" formation and dynamic properties of strongly nonideal systems of charged diamagnetic particles confined in a cusp magnetic trap have been studied. In our first experiment the principal possibility of such investigations with graphite particles of micron size has been shown. In this communication we present new experimental results obtained in late 2014, their theoretical explanations and numerical simulation.
In this experiment, we have used new replaceable containers with advanced diagnostics in which glassy cells comprise number of particles on the order of magnitude larger ($\sim 10^4$). And now the electric potential on the central electrode in the cell relative to the outer one can vary from 0 to 150 V (instead of 0 to 24 V in old containers). We used graphite particles of size 200 and 300 μm. When the central electrode was applied maximum potential (150 V), an intensive expansion of graphite particles from the cluster to the cell walls started. The average expansion velocity of the particles reached several cm/s. The process of expansion continued about 5 s until the complete disintegration of the cluster. We have performed corresponding estimations and suggest an interpretation of the observed processes. Numerical simulation of the experimental phenomena is also represented. This work was supported by the Russian Science Foundation (project No. 14-50-00124).

Ionization instability of the elongated dusty cloud in the gas discharge uniform positive column under microgravity conditions

Zobnin A V[1,@], Usachev A D[1], Lipaev A M[1], Petrov O F[1], Fortov V E[1], Pustylnik M Yu[2], Fink M A[2] and Thomas H M[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Research Group for Complex Plasmas, German Aerospace Center, Münchener Straße 20, Weßling 82234, Germany

[@] zobnin@ihed.ras.ru

A new kind of the dusty plasma instability was observed in the joint Russian-European "Plasma Kristall–4" space experiment on board of the International Space Station. A cylindrical dust particle cloud of 0.9 cm inner diameter with a length of 20 cm was formed in the uniform positive column of dc discharge operating in polarity switching mode (dc/ps-mode). The discharge operated in the glass tube of 3 cm inner diameter with a total length of 85 cm filled by argon at a pressure of 0.5 mbar. The dc/ps discharge was operated at 1 mA with the polarity switching frequency 250 Hz. During the experiment, all the dust particles vibrated synchronized in the same phase in the direction perpendicular to the tube axis with a frequency of 24 Hz and a peak-to-peak amplitude of 0.2 mm. The vibration was attended by discharge glow fluctuation. The nature of the cloud vibration is discussed. This work was supported by the Russian Science Foundation under the grant 14-12-01235. The authors acknowledge ROSCOSMOS, International Space Station, and cosmonaut Gennadiy Padalka for their support in performing of the present experiment.

Molecular-dynamic simulation of the formation and destruction of Coulomb clusters of diamagnetic particles in a cusp magnetic trap under microgravity conditions

Myasnikov M I[1,@], Dyachkov L G[1], Petrov O F[1], Vasiliev M M[1], Fortov V E[1], Savin S F[2] and Serova E O[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Korolev Rocket-Space Corporation "Energia", Lenin Street 4a, Korolev, Moscow Region 141070, Russia

[@] miasnikovmi@mail.ru

For the investigation of strongly coupled Coulomb systems of diamagnetic (graphite) particles in cusp magnetic field under microgravity conditions the experimental setup with the stable-levitation region about 400 cm^3 and magnetic field gradient up to 0.04 T/cm was produced. A cusp magnetic field is generated by two coils placed on the same axis, in which currents circulate in the opposite directions. Experiment "Coulomb crystal" were carried out onboard of the International Space Station with graphite particles of micron size placed in the middle of the replaceable container within a cylindrical glassy cell filled with argon at atmospheric pressure. Charging of the particles was carried out using a central wire electrode that passed along the axis of the cell. The electric potential of the central electrode can be increased up to 150 V. When we applied such maximum potential, the cusp magnetic trap can not confine the graphite particles and the cluster starts to break down. We have performed molecular-dynamic simulation of the cluster formation in the cusp magnetic trap and then its destruction in electric field. For simplicity we take the number of particles in the simulations to be less than that in the experiment ($\sim 10^4$). However results of our simulations are in a good qualitative agreement with observations.
This work was supported by the RFBR project 14-02-31226.

On the levitation of dust particles in a sheath of electron-emitting surface

Lisin E A[1,@] **and Kuznetsov I A**[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Space Research Institute of the Russian Academy of Sciences, Profsoyuznaya 84/32, Moscow 117997, Russia

[@] eaLisin@yandex.ru

The surface of the Moon, as well as the surface of any space body without an atmosphere, is subjected to the solar wind and ultraviolet radiation. As a result, a charge appears on the surface and electric fields near it are induced. Dust particles from the lunar regolith occurring in the near-surface plasma can levitate over the surface, forming dusty plasma clouds. One of the main problems of future missions to the Moon is associated with lunar dust.

In order to gain a better understanding of mass transfer processes occurring on surfaces of the moon and other atmosphereless celestial bodies it is necessary to conduct physical simulations in a laboratory. Usually, when the UV impact on dust particles is experimentally studied, dust levitation is provided by electric fields of a non-photoemission nature [1] or is not observed at all.

In this study we theoretically defined conditions under which levitation of various samples of dust in a sheath of electron-emitting surface irradiated with ultraviolet source is possible. Different sheath potentials were considered. It was shown that levitation of dust particles in a photoinduced sheath is possible only when directed UV radiation incident at an angle to the surface. The range of permissible angles and the maximum size of levitating particle were determined depending on the UV source power and the composition (wavelengths) of radiation, as well as on the photoemission properties of the particles and the substrate.

This work was supported by the Ministry of Education and Science (MK-7932.2015.8) and RFBR (15-32-21159).

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The effect of thermal fluctuations on the stability of particle chain-like structure

Lisina I I[@], Lisin E A and Vaulina O S

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] irina.lisina@mail.ru

r we present a study of the effect of thermal fluctuations on the stability condition for particle chain-like structure immersed in the non-isotropic plasma media. Numerical and theoretical investigations performed for the two vertically arranged particles with an anisotropic interaction, similar to an interaction due to effect of ion focusing observed in laboratory experiments with complex plasma. The obtained ratios are useful for the analysis of the dynamics of systems with different nepoparnymi interactions such as gyroscopic forces (e.g., Lorentz force), the inertia force in the inertial and non-inertial (e.g. dalamberova and Euler inertial forces), as well as other cases when the interaction is nonreciprocal.

Surface modification of charged dust particles in hybrid plasma

Gurtovoy S A[1,2,@], Statsenko K B[1,2], Vasiliev M M[1,2], Petrov O F[1,2] and Ryabov I A[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] skrafy@bk.ru

Creating composite materials is very important in various fields of science and technology. They find wide application in engineering and medicine. One of the ways to create composite materials is surface modification of microparticles.
The task of covering of the surface of powders with complex homogeneous films is not easy. The main difficulty is the size of particles that should be covered. One should control the uniformity of the obtained film, the parameters of covering (thickness, composition, etc.) and the adhesion of the coating. Creation of complex and multi-layer coatings is also actual and difficult problem.
In this work, the powder particles are trapped levitating in plasma of rf discharge during the process of sputtering. We use the energy of electron beam to heat and spray the material of the target.
We present the examples of coatings and materials obtained with the help of our technique and examine their properties and prospects of this method of coating.

Dusty clusters in cryogenic liquids

Karpyshev P A[1,2,@], Vasiliev M M[1], Petrov O F[1] and Michurina I A[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] pavel.karpyshev@phystech.edu

The study of stable Coulomb systems—ensembles of particles carrying a charge of one sign and experiencing the mutual Coulomb repulsion—is a matter of great interest. This paper studies the behavior of dust clusters of charged particles at cryogenic temperatures. This work studies superconducting particles submerged into liquid nitrogen that are held in place by inhomogeneous magnetic field. A well-known method of retention based on diamagnetic levitation of various bodies, including biological ones, in an inhomogeneous magnetic field, the so-called "magnetic well", is used.
The main element of the experimental setup is the optical helium cryostat with operating temperatures in the range from 1.8 to 273 K. Clusters of charged particulates are formed in the magnetic trap inside the cryostat. The powder used consists of polydisperse $YBa_2Cu_3O_7$ particles. The dust is illuminated with a laser beam. To prevent boiling of the cryogenic fluid the shaft of the cryostat is pumped with a turbomolecular pump. The highlighted particulates are recorded using high speed video camera through the optical window of the cryostat. The coordinates of the dust particles and the profile of their velocities is determined using image processing software. The particles are charged using an electric probe with a potential of 2000 V. The charge on the particles can be either positive or negative, and was $107e$ during the experiment. The formation of strongly correlated structures consisting of about 103 particles was observed. The average interparticle distance equal to 475 μm was calculated on the basis of experimental data. Estimates of the nonideality parameter $\Gamma \sim 107$ and the Lindemann parameter $L \sim 0.03$ were conducted, which are specific to crystalline or glassy highly correlated systems.

Nanoparticle confinement by the linear Paul trap

Lapitsky D S[@] and Filinov V S

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] dmitrucho@yandex.ru

The purpose of this work is studying of nanoparticle confinement by alternating electric field of the linear Paul trap in air. In the previous works [1–3] the possibility of confinement of the Coulomb systems of charged microparticles in air at atmospheric pressure by linear Paul traps was demonstrated. The regions of charged microparticles confinement in a wide range of parameters were determined. The aim of this work is to expand studying of particle capturing to the area of nanoparticles. Due to the small nanoparticle size the effect of slippage in the gaseous medium will appear and the Cunningham-Millikan correction factor C_k should be taken into account that will change the capturing parameters for nanoparticles in comparison with the capturing of micron sized particles. The equation of motion of nanoparticle is described by the Langevin equation:

$$m_n \frac{d^2 r}{dt^2} = F_t(r) - 6\pi \frac{\eta}{C_k} r_n \frac{dr}{dt} + F_b + F_g \qquad (1)$$

where r is the vector of nanoparticles, m_n and r_n are nanoparticle mass and radius, $\eta = 18.2$ μPa s is the air dynamic viscosity, F_t(r) is the force of interaction of nanoparticle with the trap electrodes, F_b is the stochastic Gaussian delta correlated force of collisions of neutral particles with the nanoparticle, F_g is the gravity force.

The work was done by the financial support of the Russian Science Foundation via grant 14-50-00124.

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The confinement region of charged particles trapped by microparticle electrodynamic ion trap

Syrovatka R A[@], Deputatova L V, Filinov V S, Lapitsky D S, Pecherkin V Ya, Vasilyak L M and Vladimirov V I

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] syrovatkara@gmail.com

The first demonstration of the charged particles confining using microparticle electrodynamic ion traps (MEITs) has been performed in 1955 [1]. The possibility to confine a levitating particle turned up very useful to measure the detailed properties of individual charged particles. Besides individual particles, MEITs can also trap large numbers of charged particles that self-organize into Coulomb crystalline structures [2]. Previously [2], numerical simulations of the motion of particles affected by time-varying trap electric fields have been performed and such parameters of the trapped particles confinement region as the dynamic viscosity of the gas medium, particles charge to mass ratio and frequency and amplitude of AC voltage applied to the trap electrodes have been determined.
In this paper, the trapped particles confinement region has been determined experimentally. The experimental setup was described in paper [3]. The confinement region was determined in the following way. At the first stage the trapped particle charge and mass were measured and at the second stage the AC voltage frequency were varied until the particle fell out of the trap.

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Dynamics of microparticle Coulomb structures in linear electrodynamic traps with different numbers of electrodes

Vladimirov V I[@], Vasilyak L M, Syrovatka R A, Pecherkin V Ya, Lapitsky D S, Filinov V S and Deputatova L V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vld@ihed.ras.ru

Electrodynamic quadrupole traps are used for creation of self-organized Coulomb crystalline structures [1]. In paper [2] parameters range which is required for confinement of an ensemble of charged microparticles in a linear quadrupole trap has been determined using numerical simulation methods. In this paper using numerical simulation methods we obtained information about dynamics of Coulomb crystalline structures in linear quadrupole traps with different numbers of electrodes. The two, four, six and eight-electrode traps have been examined. Experimental investigations were performed for vertically oriented traps. In this case the effects of gravity on radial particles distribution in the traps are absent and radial symmetry of the dust structure takes place. The experiments were performed for the two, four and eight-electrode traps. Particles oscillated along the field lines. The possibility for Coulomb structures localization in a certain area of space has been shown.

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Electric parameters of dc discharge in neon at cooling

Vasilyak L M, Polyakov D N[@] and Shumova V V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] cryolab@ihed.ras.ru

The experimental study of the behavior of current–voltage characteristics (CVC) of the discharges under gas cooling is necessary for the development of a model of gas-discharge plasmas at low and cryogenic temperatures. The electric field strength is one of the fundamental characteristics of plasma, which determines the intensity of ionization processes in plasma. The measurement of change in electric field strength in dusty plasmas is the important tool in studying its properties and the processes of its self-organizing. The voltage drop of the total discharge and the CVC of a positive column were measured in the 16.5 mm i.d. discharge tube of 200 mm length cooled by a stream of gaseous nitrogen in optical cryostat. The temperature of a walls of the discharge tube was adjusted in the range 77.4–300 K. The measurements were carried out in a pressure range of 18–187 Pa, and discharge current of 0.1–3.5 mA. It was found that the longitudinal electric field strength in the positive column is increased slightly with cooling, but there is a significant increase in discharge voltage drop in the temperature range 160–120 K. The increase in the discharge voltage drop is not equal to an increase in voltage drop on the positive column. The dependence of the electric field strength on pressure at a fixed discharge current is nonmonotonic. It was observed that with increase in pressure or decrease in gas temperature the CVC of normal glow discharge slightly increase with increasing current, which may be due to the higher mobility of the resulting molecular ions of neon. It was revealed that at the transition from room temperature to temperature of liquid nitrogen, the strength of the reduced electric field decreases, and the transition to the normal glow discharge shifts to smaller discharge currents for the same values of the reduced pressure.

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Glow discharge in neon with dust-void

Shumova V V[@], Polyakov D N and Vasilyak L M

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] shumova@ihed.ras.ru

The formation of dust-free regions (voids) in dust clouds sustained in a glow discharges was observed in air, air–argon mixtures [1–3], helium [3, 4] and neon [5]. In this study, we simulate the parameters of neon glow discharge with dust-voids. The simulations are based on the drift-diffusion model of the uniform glow discharge positive column in neon with dust particles [6]. The formation, drift, diffusion and losses of electrons, ions and metastable neon atoms were considered in plasma bulk, on the discharge tube walls and on the dust particle surface. The distribution of dust particles in the discharge was set by a step function with a cavity inside, corresponding to the void radius, and the concentration of dust particles was close to that observed in experiments [5]. Simulations were carried out with the experimentally obtained values of the discharge parameters corresponding to the transformation of homogeneous dust structures to the structures with dust-void. The radial distributions of plasma particles, the radial and longitudinal components of the electric field were calculated. The significant difference of the discharge parameters with and without dust-voids was demonstrated.

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The electrical characteristics of dc discharge with microparticles

Polyakov D N, Shumova V V[@] and Vasilyak L M

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] shumova@ihed.ras.ru

Charged microparticles and dust structures, formed in the gas-discharge plasma, change the properties of the surrounding plasma as a result of the dissipation of energy and losses of plasma particles on the surface of dust particles or as a result of the emission from the surface of dust particles. The experimental results are presented on the change in the longitudinal electric field strength with the introduction of micron-sized dust particles in the plasma of the positive column of a glow discharge in neon. The experimental results are compared with the simulations in frames of drift-diffusion approximation. The analysis of the particle charge is represented to explain the interaction of microparticles with a plasma of a discharge. In the case of a large number of dust particles in the discharge they act on the plasma collectively as a dust structure. At the location of a dust structure the gas conductivity decreases, which causes a redistribution of the electric current density over the cross section of the discharge and increase in the longitudinal electric field strength. With the increase in the concentration of dust particles in the structure, the increment of the longitudinal electric field strength related to a single dust particle is reduced, which is reflected in change the dust particle charge. With increasing the dust particle number density in the dust cloud, the individual charge of dust particles decreases, however, the charge volume density in a discharge increases. The adequate regard of the parameters of discharge with dust particles is important for the simulation of plasma traps for dust particles.

Spark breakdown in uniform electric field in the presence of dust particles

Pecherkin V Ya[@], Vasilyak L M and Vetchinin S P

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vpecherkin@yandex.ru

The physical processes leading to formation of high conductivity plasma channels at formation of electric breakdown in disperse mediums are of interest to the solution of various tasks, such as formation of electric discharges in dust clouds and so on.
Complexity of research of electric discharges in such objects is connected with unpredictability of their emergence in time and space. Existence of a disperse phase essentially influence on the formation of electric breakdown. Efficiency of interaction of electric field with substance in the dispersed state is much higher that is connected first of all with polarization of macroparticles and their charging that causes strengthening of electric field on the interphase boundary. Intensity of electric field in such mediums significantly goes down that facilitates development of intensive ionization and formation of spark channels. Mechanisms of development of breakdown in disperse environments are not revealed so far and still there is no the finished theory of spreading of pulse currents. It is connected with complexity of diagnostics of the proceeding processes, a lack of experimental data and ambiguity of their interpretation.
Experimental studies were carried out in uniform electric field with flat electrodes. Particles were thrown in the volume of an interelectrode interval. Emergence and development of an electric discharge was registered the high-speed camera. The electric discharge was initiated on particles inside the interval. It was revealed that in the presence of solid dielectric or metal particles the relay mechanism of development of breakdown when breakdown develops from particle to particle, resulting in the entry of gap. Without particles breakdown of gap did not arise. Thus, the presence of dust particles reduces the threshold of the breakdown development, and defines the dynamics and spatial characteristics of the spark channel.

Breakdown of a conducting fluid with microbubbles from a sharp tip anode

Vetchinin S P[@], Vasilyak L M, Pecherkin V Ya, Panov V A and Son E E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] uvlightsvp@yandex.ru

Experimental research on electrical breakdown and spark channel propagation in a conducting fluid with microbubbles from a sharp tip anode under high voltage pulse has been performed. Investigation was provided in 15% solution of isopropyl alcohol in tap water at different air microbubbles volumetric content (3 and 10%). In contrast to the homogeneous fluid the presence of a large number of microbubbles in a conducting fluid increases the rate of the plasma channel propagation velocity by several times due to the ionization of the gas in the microbubbles along the plasma channel path. The microbubbles also causes an increase in the current when the discharge gap is circuited. The observed rate of the channel propagation in the microbubbled fluid ranges from 4 to 12 m/s indicating thermal mechanism of the spark channel development. It has been shown that the breakdown of a conducting fluid with air microbubbles can develop through the thermal mechanism when 10–20 kV pulse voltage with millisecond duration is applied to the sharp tip anode.

The breaking of two-dimensional nonlinear plasma oscillations

Frolov A A[1,@], Chizhonkov E V[2] and Milyutin S V[3]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Lomonosov Moscow State University, Leninskiye Gory 1, Moscow 119991, Russia
[3] Limited Liability Company "Rock Flow Dynamics", Schelkovskoe Highway 9, Moscow 105122, Russia

[@] frolov@ihed.ras.ru

The stability problem for spatial structure of plasma oscillations in the process of their dynamics is studied in the paper analytically (by perturbation methods) and numerically. Applying the method of perturbations, we studied the stability of the spatial form of two-dimensional oscillations for the breaking moment. It is shown that if the initial perturbation possesses an axial symmetry, then the breaking (i.e., the singularity of the electron density function) appears simultaneously on a circumference having a certain nonzero radius. If sections of the initial perturbation of the electron density are ellipses, then the singularity appears also simultaneously, but only at two points. The qualitative change in the final breaking pattern does not depend on the quantitative deviation of the ellipse form a circumference, implies that the electron density turns to infinity at only two points. The two-dimensional numerical simulation of the indicated effect (instability of the spatial structure of the electron density function) was performed by the method of the second order of accuracy in the Euler coordinates developed by the authors and admitting an implementation by means of explicit formulas. We present the results of calculations performed in the Supercomputing Center "Chebyshev" of the Lomonosov Moscow State University on the base of a hybrid parallel code. The results are in a good agreement with analytic calculations and the results of computations with one-dimensional models. It seems that the obtained results can be important for correct interpretation of field experiments.

Dusty plasma of non-self-maintained discharge in inert gas at low pressures

Andryushin I I[@] and Zherebtsov V A

Joint Stock Company "State Scientific Centre of the Russian Federation—Institute for Physics and Power Engineering named after A I Leypunsky", Bondarenko Square 1, Obninsk, Kaluga Region 249033, Russia

[@] i.andryushin@gmail.com

An overview of the sequence of works on investigation of non-self-maintained discharge dusty plasma and its instability is presented. The discharge is maintained by a beam of protons and is using for simulation of nuclear-induced plasmas and studying of dust plasma structures [1, 2].

The study was carried out in four main steps: (i) estimation of the main parameters of non-self-maintained discharge supported by a proton beam in inert gas under conditions when steady-state and non-steady-state ordered dust structures are formed [3]; (ii) studying of the dusty plasma stability at a low pressure of inert gas [4]; (iii) analysis of physical mechanism of instability [4] (so called recombination instability) which leads to the separation of the plasma into the regions with high and low densities of dust particles [1, 2]; (iv) analysis of the dependence of instability development conditions on the parameters of the discharge and investigation of the nonlinear stage of the perturbations development.

The studies were conducted with the financial support of the Russian Foundation for Basic Research and the Government of the Kaluga region (grants No. 12-02-97521 and No. 14-42-03006).

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Diagnosis of low temperature dielectric barrier discharge plasma at atmospheric pressure

Bryuzgin S V[1,2,@], Vasiliev M M[1] and Petrov O F[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] nikel.26@mail.ru

For a long time, the using of plasma in medicine has been bound with its thermal effect upon exposure on the treated surface. Recently, the interest in the study of plasma with the temperature no more than 40 °C has increased due to a number of possible applications: sterilization, wound healing, cell dividing and others. In particular, an article [1] presented the results of microbiological studies, which show the effectiveness of the impact of low-temperature helium plasma dielectric barrier discharge on pathogenic bacteria.
In this work, the results of the optical and probe diagnostics of low temperature dielectric barrier discharge plasma are provided. The plasma is produced by creating a plasma channel in a flow of helium at atmospheric pressure. Spectra emission in the wavelength range 220–900 nm were obtained. By analyzing spectral measurements the main plasma components were determined. Depending on the distance from a plasma source were measured concentrations of active components such as O_3, NO_2 and NO by means of the gas analyzer.

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Optimization of the dielectric barrier discharge efficiency to produce synthetic jets

Bocharnikov V V[@], Volodin V V and Golub V V

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vova.m.bocha@gmail.com

The dielectric barrier discharge of symmetric actuator generates a synthetic jet that is perpendicular to the surface of the actuator. You can set the actuator on the lower surface of the wing of an aircraft near the trailing edge. Then the synthetic jet will perform the function of the flap. Thus it is possible to significantly increase the lift force [1]. At the same time drag varies insignificantly [2]. Velocity and specific impulse of the incident flow exceeds the value that could be achieved in a synthetic jet. Consequently, for successful application of dielectric barrier discharge is necessary to find a mode in which the electric discharge energy most efficiently converted into the kinetic energy of the jet. In the present paper we investigated the relationship between the specific thrust of synthetic jet and electrical discharge power. Experimentally it was found dependences of specific thrust for power on the frequency of alternating voltage and the value of ballast resistance. According to the study was proposed energy-efficient mode of symmetric plasma actuator. In this energy losses are minimized and the synthetic jet thrust reaches its maximum value at a predetermined amplitude of the alternating voltage.

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Characteristics of extensive atmospheric discharge

Agafonov A V[1], Baidin I S[1], Letunov A A[2], Oginov A V[1,@], Rodionov A A[1] and Shpakov K V[1]

[1] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

[2] Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova 38, Moscow 119991, Russia

[@] oginov@lebedev.ru

Research of spark discharges were carried out on the installation ERG LPI (1 MB, 60 kJ, 150 ns rise time) [1]. Registration of hard radiations in real time was conducted using pulse photomultipliers, stacked with plastic scintillators. The radiation in the visible region of the spectrum with the development of an extensive discharge in air in the interelectrode space of 500–600 mm in length carries information about the parameters of streamer–leader stage of the discharge, the discharge channel interaction with the electrode material, a stage of relaxation after the decay of the plasma channel of the discharge current. For registration of emission spectra were used AvaSpec 3648 spectrometer with a resolution of 0.3 nm in the wavelength range from 370 to 920 nm and AvaSpec 2048 with a resolution of 1.3 nm in the wavelength range from 185 to 750 nm. Emission was collected integrally from the cross-sectional area substantially remote from both electrodes. Temporal measurements conducted by monochromator with photomultiplier. The visible spectra obtained are similar to those of the natural linear lightning obtained in [2], in the presence of the lines of N II ion in the shorter wavelengths range, and in the range of more 700 nm—lines of atomic nitrogen and oxygen. The electron temperature was about 3 eV. This corresponds to a significant degree of ionization.

This work was supported by grant No. 16-12-10497 from the Russian Science Foundation.

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The numerical solutions of the pre-breakdown electro-hydrodynamic equations at a liquid insulators

Apfelbaum M S and Doludenko A N[@]

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] adoludenko@gmail.com

The liquid insulator under high voltage reveals well-known features of its behavior, that is concluded in deviation of the current–field dependence from Ohm's law. In this work we study the pre-breakdown behavior of liquid insulator on the base of our model. According to this model the liquid dielectric is analogous to the weak electrolyte. The partial dissociation of its molecules takes place. The volume concentrations of the ions $n_\pm$ and the impurities n_p are supposed to satisfy the following conditions:

$$\left\{ \begin{array}{rcl} n_\pm & \ll & n_a, \\ n_p & \ll & n_a, \end{array} \right. \tag{1}$$

n_a is the concentration of neutral particles (molecules). If we suppose, that the ion mobilities are equal for the liquid insulator ($b_+ = b_- = b$), we will obtain, using the equation (1):

$$\left\{ \begin{array}{l} \frac{\partial q}{\partial t} + (\vec{V}, \nabla q) - \frac{k_B T b}{|e|} \Delta q + (\vec{E}, \nabla \sigma) = -\frac{q\sigma}{\varepsilon\varepsilon_0}, \Delta\phi = -\frac{q}{\varepsilon\varepsilon_0}, \\ \frac{\partial \sigma}{\partial t} + (\vec{V}, \nabla \sigma) + b^2 (\vec{E}, \nabla q) - \frac{k_B T b}{|e|} \Delta\sigma - \frac{\sigma_0^2}{\varepsilon\varepsilon_0} \exp(\beta\sqrt{|\vec{E}|}) = -\frac{\sigma_0^2}{\varepsilon\varepsilon_0}, \end{array} \right. \tag{2}$$

where t is the time, V is the hydrodynamic velocity of neutral component and approximately equal to the velocity of the whole mixture. The coefficient in first exponent in the equations (2), is depended on absolute temperature T, ion charge e and dielectric permittivity of the considered medium. Numerical calculations of the components V, caused by pre-breakdown electric field are provided with use of the Navier–Stokes equations.

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High-pressure ignition plasma torch for hypersonic cruise vehicles aerospace testing

Yusupov D I[@], Kulikov Yu M, Gadzhiev M Kh, Tyuftyaev A S and Son E E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] spt_yusupov@mail.ru

To extend the operating range of aerodynamic tunnel plants aimed for hypersonic cruise vehicles testing one can use combustion gases for primary flow preheating. Ignition devices which in particular are powerful spark plugs have to operate in severe environment characterized by very high breakdown voltage due to high pressures (≈ 70 bar) that exceeds 60 kV going beyond the limits in which the Paschen's law is valid and has a serious variance, accompanied by the increase of the mean value due to electrodes conditioning. High fuel mixture flow rates (up to 200 kg/s) require spark current increase that leads to accelerated deterioration of spark plug electrodes. The high-pressure plasma torch poses a reasonable alternative to spark plug ignition of combustive mixture in wind tunnel facilities. We performed the analysis of the arc ignition systems, including those involving the breakdown voltage reduction due to an alternating electric field and high-frequency field application. Basing the equilibrium dissociation and ionization equations we calculated the thermal properties of the nitrogen plasma at pressures up to 100 bar. In addition, high pressure nitrogen plasma electrical conductivity has been determined up to temperature $T = 120000$ K and manifested reasonable agreement compared to the results of other researchers. Utilizing the specific enthalpy temperature dependence the power demand of electric arc have also been estimated as the function of the flow rate and the bulk temperature of the gas. As part of the experimental studies we have tested various technical solutions and measured the performance data that ensured a stable ignition and operation of the plasma torch at high pressures.

Hypersonic cruise vehicle shock-compressed layer radiative properties investigation

Kulikov Yu M[@], Savitsky D V and Son E E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] kulikov-yurii@yandex.ru

As hypersonic fluid flow static temperature exceeds $T = 1$ eV, the radiation becomes significant occupying 15% share in the overall heat transfer. The present paper delivers software module verification results intended for calculation of the intense radiative heat transfer in the shock-compressed layer at the hypersonic cruise vehicle surface utilising the multigroup absorption coefficient approximation and plane layer radiative model in the wide range of temperatures $T = 2000$–20000 K and pressures $p = 10^{-3}$–10^{2} bar. The module implements generalized multigroup or standard multigroup spectrum approximations and normal radiative flux calculation routine based on the plane layer model. The generalized multigroup approximation fits the true spectrum more accurately compared to the standard multigroup approximation if resonant skeleton structure coincides (or is very similar) to base spectrum one. Otherwise, the approximation accuracy drops sharply. Therefore, standard multigroup approximation is more consistent being applied to wide temperature range calculations with a possible increase of spectral groups number up to $N = 16$. The convergence rate of multigroup and generalized multigroup approximations varies significantly on the different spectal subranges for the selected reference spectrum. However, comparing the value of the integral radiative heat flux we showed that generalized multigroup approximation overestimates the total heat flux by 40%, and the standard one—by 20% compared the true spectrum. Thus, the latter appears to be more preferable.
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Fine structure of dielectric barrier discharge

Panov V A[@], Vasilyak L M, Pecherkin V Ya, Vetchinin S P, Saveliev A S, Kulikov Yu M and Son E E

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] panovvladislav@gmail.com

The dielectric barrier discharge could be a promising tool for controlling sprawling fungi at the International Space Station. In the present study we investigated the fine spatial structure of the barrier discharge at the alternating voltage. We used a classical electrode system in which HV electrode is placed on the surface of a thin dielectric layer (200 micron of PTFE), and the ground electrode is encapsulated in a body of the Plexiglas substrate. The voltage source consists of an amplifier with a high voltage coil. It provides a sinusoidal output voltage of 11 kV range (5.5 kV of amplitude) at frequency of 4.5 kHz. Visualization is conducted by means of the following system: microscope Questar QM1, image intensifier LaVision IRO, and a high-speed camera Photron SA-4. System timing is set so that the camera records one and the same phase in successive periods of voltage signal. Ten successive phases of the discharge were studied in the present investigation. The following experimental facts were established in the course of the study: 1) intense glow discharge was registered only in the first and third quarters of the period of voltage signal; 2) the characteristic length of the field of the spread of the plasma streamer discharge phase as compared with this value for the diffusion phase of the discharge are3.1 mm and 2.5 mm respectively; 3) the plasma channels elongation is observed during the whole time of voltage rise time; 4) light emission completely disappears almost immediately after the start of reducing the absolute value of the voltage; 5) the characteristic length, after which the intensive branching of streamer channel starts is 400-600 micron; 6) at the diffusion stage plasma region has a torch-like shape with the full opening angle of the order of 30-60 degrees.

Accessible parameters of high-current channel at high pressure gas

Bogomaz A A[1], Pinchuk M E[1,2,@], Budin A V[1], Leks A G[1], Leont'ev V V[1], Pozubenkov A A[1] and Kurakina N K[1,2]

[1] Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, Russia
[2] Peter the Great Saint-Petersburg Polytechnic University, Polytechnicheskaya 29, Saint-Petersburg 195251, Russia

[@] pinchme@mail.ru

Results of experiments in hydrogen for discharge with current amplitude up to 1 MA, current rise rate $\sim 10^{10}$ A/s, and at initial pressure up to 30 MPa are presented. It was considered a physics mechanism of most deep channel contraction on current rise stage of the discharge. Also experimental estimations of plasma channel terminal parameters at contraction are described.
Original electric and magnetic probes [1] were designed and created for diagnostics. Also it were used an photostreak analysis [2] and soft x-ray registration [3] from the discharge channel.
The discharge was initiated by copper wire explosion. Discharge chamber was designed with axisymmetric geometry. Capacity of energy storage was changed. It was 1.2, 2.4 or 4.8 mF. Charging voltage was varied from 1 to 15 kV. Energy input was up to 300 kJ. Minimal temperature and maximal channel radius were determined at the time of maximum contraction. Estimations of the temperature and radius boundaries are 2×10^{-3} cm and 42 eV correspondingly. A comparison between the contraction rate of plasma channel with metal vapor and discharge with a predominance of hydrogen plasma was made. A higher speed for the metal plasma confirms the radiative mechanism of contraction.

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Energy deposition in discharge chamber of lightning protection multichamber system

Pinchuk M E[1,2,@], Budin A V[1], Kumkova I I[1], Bogomaz A A[1], Sivaev A D[3,2], Chusov A N[3] and Zaynalov R I[3]

[1] Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, Russia
[2] Peter the Great Saint-Petersburg Polytechnic University, Polytechnicheskaya 29, Saint-Petersburg 195251, Russia
[3] Streamer, Electric Company Inc., Office 17N, Nevsky Prospect 147, Saint-Petersburg 191024, Russia

[@] pinchme@mail.ru

The experimental results of energy deposition distribution measurements along discharge chamber of lightning protection multichamber system in initial stage of discharge process aimed to model lightning current impulse up to 10 kA are presented. A multichamber system is a series connection of discharge chambers. Preliminary data for current 10 kA is reported in [1]. In paper [2], shock wave velocity measurements had been made for similar system. But the velocity exceeded theoretical estimation [2]. This effect was explained by the interaction of the gas jet from discharge volume with the shock wave [2]. According to our experiments the shock wave formation occurs during the breakdown phase between electrodes located at the bottom of discharge chamber. The consequent energy deposition during discharge development goes in the whole volume bounded by shock wave front. Thus, the shock wave recieves additional energy from the discharge during all its way out of chamber.

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High current electric arcs above the In-Ga-Sn eutectic alloy

Klementyeva I B[1,@] and Pinchuk M E[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, Russia

[@] ira.klementyeva@mail.ru

Plasma technologies are widely used in the processing industries. All the variety of constructive devices can be divided into that with plasma torches and free burning high-current arcs. The most promising method of waste recycling is technologies using the electro-arc reactors. In comparison with plasma torches, they have a grater capacity, but at the same time have a number of problems with the stability of the electric arc.

The paper is devoted to the investigation of the high current arc discharges of atmospheric pressure burning above the free surface of the electro-conducting material that is initially in liquid aggregate state. The main tasks of the work are: to investigate the processes of the ignition, formation and evolution of the high-capacity pulsed arcs, DC arcs and AC arcs of industrial frequency and to determine their parameters under the conditions of consideration.

The test section is a cylindrical container of 10 cm diameter and 4 cm depth filled with the eutectic alloy of In-Ga-Sn, and rod steel electrode of 0.76 cm diameter with hemispherical tip. The electric current in the circuit is organized by the generator of current pulses of 25 kV, 30 kA and 300 mks duration for the regimes with the high-capacity pulsed arcs, by the oscillating circuit of 10 kV, 10 kA, 10 ms duration and 50 Hz for the regimes with the AC arcs, by the accumulator batteries of 25 V and 1.5 kA for the regimes with the DC arcs. The data reflecting the processes in the system with the rod electrode initially dipped on a depth of its tip into the melt– the deformation of the contact surface, ignition and evolution of the electric arcs,–and its parameters were obtained in the experiments.

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On the mechanism of retrograde motion of vacuum arc cathode spot in external magnetic field

Barengolts S A[1,2,@], Mesyats V G[1] and Tsventoukh M M[2]

[1] Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova 38, Moscow 119991, Russia

[2] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

[@] sb@nsc.gpi.ru

The phenomenon of a retrograde (anti-Ampere) motion of the cathode spot (CS) of vacuum arc in an external magnetic field parallel to the cathode surface is among the most intriguing and difficult to explain effects in the physics of vacuum discharge. The interest in this phenomenon was related, besides its exotic character, to the idea that understanding of the mechanism of this motion would provide a key to constructing a theory of the CS of vacuum arc. However, the time passed and the number of models suggested to explain the retrograde motion exceeded the number of the proposed mechanisms of operation of the CS proper. The report describes the main physical processes that lead to the retrograde movement of the cathode spot of a vacuum arc in the external tangential magnetic field. Application of a magnetic field leads to an asymmetry in the distribution of the magnetic field at the boundary of cathode plasma. The maximum value of the total magnetic field (self + external) is reached on the reverse side of spots relative to the direction of the force Ampere. Here, the maximum magnetic pressure and concentration of the cathode plasma. At the moment of death spots in this direction is prevailing emission of the plasma and, as a result, the ignition of a new spot. A statistical model of the motion of the cathode spot in the external magnetic field is developed.
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On the cyclic behavior of the cathode spot cells in a vacuum arc

Mesyats V G

Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova 38, Moscow 119991, Russia

sabarengolts@mail.ru

The cathode spot of a vacuum arc consists of cells, each operating for a certain time referred to as a cycle. Within this time, a microexplosion occurs on the cathode surface, resulting in the formation of liquid metal, vapor, and plasma of the cathode material. The plasma blob ejected by a cell is called an ecton. In this paper, it is shown that the cycle involves three phases: heating, burning, and cooling of the cathode material, rather than two ones, as believed earlier. For a copper cathode, the first and third phases last about a nanosecond, whereas the duration of the second phase is of the order of ten nanoseconds. During the cooling of one cell and the heating of another, a voltage pulse arises between the cathode and the anode. As the formation of cathode cells is due to the plasma–liquid-metal interaction in the presence of a cathode potential, this voltage pulse provides for the self-sustainment of the discharge.

Preparation and properties of a composite SiC/multi-wall carbon nanotubes synthesized in the plasma jet

Shavelkina M B[1,@], Amirov R Kh[1], Kelina I Yu[2] and Golubeva N A[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Obninsk Research and Production Enterprise "Technologiya", Kievskoye Shosse 15, Obninsk, Kaluga Region 249031, Russia

[@] mshavelkina@gmail.com

Due to unique combination of their physical and chemical properties the high-temperature ceramics based on silicon carbide are widely in demand in mechanical engineering, nuclear energy, defense, metallurgy, food, chemical, oil and oil refining industries [1]. Because of a high fragility of SiC ceramic materials the composites based on it have the greatest prospects. The report discussed methods for the preparation and properties of silicon carbide composites containing thin multi-walled carbon nanotubes (CNTs). CNTs obtained by pyrolysis of acetylene in helium plasma at a pressure of 350 Torr, arc current of 400 A. As the generator of plasma a DC plasma torch was used with the power of up to 40 kW and an expanding anode channel. By varying of the flow rate ratio of acetylene and helium at a constant synthesis time of 10 min were found the conditions under which the CNTs are collected into bundles. The bundle diameter is not greater than 100 nm. From the data of electron microscopy of the cleave of the modified SiC ceramic containing 1 wt.% CNTs, there is no the unwinding of bundles and the stretching of nanotubes. In general experimental data was obtained, showing the possibility of forming a SiC/CNTs composite having both the high crack resistance and the high strength—an atypical combination for a ceramic.

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Particularity of the electrochemical behavior of the graphene materials synthesized by using dc plasma torch

Shavelkina M B[1,@], Rychagov A Yu[2] and Amirov R Kh[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Frumkin Institute of Physical Chemistry and Electrochemistry of the Russian Academy of Sciences, Leninsky Avenue 31, Moscow 199071, Russia

[@] mshavelkina@gmail.com

Rechargeable batteries, fuel cells and supercapacitors are the typical electrochemical devices. Now, instead of graphite, which has been a key component in the existing electrochemical devices, graphene can be used. The most common method of producing graphene is the reduction of graphene oxide. However, this method does not allow graphene to be completely free of oxygen and leads to the formation of graphene with a high concentration of hybridization defects. From the viewpoint of producing a low-defected graphene it is of interest to use a plasma jet synthesis method wherein evaporation of carbon-containing precursors (soot, hydrocarbons, alcohols) takes place directly in a plasma generated by a dc plasma torch. Helium, argon or nitrogen are used as plasma gasses. The optimum regime is achieved by widely varying: pressure, energy input, and relationship of plasma gas flow, a precursor and a catalyst.
Electrochemical studies of synthesized in the plasma jet graphenes show high hydrophobicity and resistance to oxidation. Their hydrophobic properties are maintained for a long time even in deep (greater than 1 V) cathode-anode polarization in sulfuric acid solution. Oxidation potentials of graphene at 1.6–1.7 V (RHE) leads to an increase in capacity by 2–3 orders of magnitude. These properties allow the use of these graphenes as carriers of catalysts for gas diffusion electrodes of fuel cells and air-metallic current sources. In addition, low defects and high electrical conductivity can be considered as promising conductive additives for electrodes in non-aqueous electrolytes.

Distributed vacuum arc with cerium oxide hot cathode

Amirov R Kh, Vorona N A, Gavrikov A V, Liziakin G D, Polistchook V P, Samoylov I S, Smirnov V P, Usmanov R A[@], Yartsev I M and Ivanov A S

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] ravus46@yandex.ru

Distributed vacuum arc with hot cathode is one of the perspective plasma sources for development of spent-nuclear-fuel plasma reprocessing technology. Experimental data is known for such type of discharges on metal cathodes. In this work discharge with cerium dioxide hot cathode was studied. Cerium dioxide properties are similar to uranium dioxide. Its feature as dielectric is that it become conductive in oxygen-free atmosphere [1].

Vacuum arc was studied at the following parameters: cathode temperatures laid between 2.0 and 2.2 kK, discharge currents was between 30 and 65 A and voltages was in range from 15 to 18 V. Power flows from plasma to cathode were estimated in achieved regimes. Analysis of generated plasma component composition was made by radiation spectrum diagnostics. These results were compared with calculations of equilibrium gaseous phase above solid sample of cerium dioxide in close to experimental conditions. Cerium dioxide vacuum evaporation rate and evaporation rate in arc were measured.

The study was supported by grant from the Russian Science Foundation (project No. 14-29-00231).

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The formation of a crater on the surface of the cathode in the explosion of micro tip

Oreshkin E V[1,@], Barengolts S A[2,1], Mesyats G A[1], Oreshkin V I[3,4] and Khishchenko K V[5]

[1] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia
[2] Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova 38, Moscow 119991, Russia
[3] Institute of High Current Electronics of the Siberian Branch of the Russian Academy of Sciences, Akademichesky Avenue 2/3, Tomsk 634055, Russia
[4] National Research Tomsk Polytechnical University, Lenin Avenue 30, Tomsk 634050, Russia
[5] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] oreshkin@lebedev.ru

Presented are the results of numerical simulation of the formation of a crater on the surface of the cathode during the explosion of micro tip [1]. The simulation was performed using the two-dimensional MHD program [2], wide-range equation of state [3] and a table of conductivity of the metal based on experimental data. It is shown that the electric explosion of micro tip with parameters typical unit ecton may form on the cathode surface of the crater with a radius of a few microns.

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Modification of the composite multi-layer oxide ceramic coating on meteoroid shielding element by compression plasma flow

Astashinski V M, Khramtsov P P, Hryshchanka U M, Chernik M Yu[@], Vasetskij V A, Shikh I A, Doroshko M V and Makhnach A I

Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus, P Brovka Street 15, Minsk 220072, Belarus

[@] Emerald_@tut.by

The aim of this work is investigation of the effect of high-energy plasma impact on meteoroid shielding element to increase their performance by improving surface physical and mechanical properties. To reach this goal, composite multi-layer coating (NiAl as a sublayer and Al_2O_3 as a top coat) was plasma sprayed on traditional material surface and then treated by high-energy qausi-stationary compression plasma jets. Compression plasma flow impact causes in a surface layer of oxide ceramics unsteady melting and recrystallization and improving the characteristics of the viscous coupling of NiAl metal layer and a layer of a solid oxide ceramics Al_2O_3. Effect of compression plasma flow causes the formation of the remelted oxide layer of 6–7 μm thickness. The method of energy dispersive x-ray microanalysis was used to study changes in elemental and phase composition, surface morphology and mechanical properties of modified shielding elements. Visual examination, photography and spectral measurements of plasma flow was made to study shape, temperature and behaviour of compression plasma jet. Ballistic tests of meteoroid shielding element were conducted with use of two-stage light-gas magnetoplasma launcher. As a result of the impact of projectile (graphite ball with a diameter of 2.5 mm and speed of 4.8 km/s) crater ($d \approx 4$ mm) appeared and part the composite coating peeled off in the vicinity of the crater, but meteoroid shielding element remained unpierced.

The investigation of heterogeneous flow generated by the direct current plasma torch

Penyazkov O G, Shatan I N[@] and Evmenchikov N L

Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus, P Brovka Street 15, Minsk 220072, Belarus

[@] inshatan@gmail.com

In the article, the two-phase flow of electric arc gas heater of the linear scheme is studied. The power of the plasma torch can be varied from 200 to 1500 kW. For stabilization of the electric arc, a magnetic coil is used. The operation of the plasma torch took place at overpressure in the discharge chamber. Injection of the powder was made near the exit of the nozzle. A powder of SiO_2 was used as a disperse phase. The size of the particles was not more than 50 μm. The dispensing device was used for the powder injection.
The technique of velocity measurement in high-temperature heterogeneous flow from the registration of flow by the high-speed camera is presented. The results of measurements indicate that the speed of the particles much lower than the speed of the gas.
The results of measuring the heat flux along the axis of the plasma torch are presented. The heat flux was measured by means of regular mode uncooled sensors with tablet type calorimeters.

Influence of surface finish on the plasma formation at the skin explosion

Datsko I M[@], Chaikovsky S A, Labetskaya N A and Rybka D V

Institute of High Current Electronics of the Siberian Branch of the Russian Academy of Sciences, Akademichesky Avenue 2/3, Tomsk 634055, Russia

[@] datsko@ovpe.hcei.tsc.ru

The main goal in the design of the load in high-current generators is to increase the time preceding the plasma generation on the electrode surface and to decrease the velocity of its expansion. The paper presents the results of the study of plasma formation on the surface of conductors at their skin explosion depending on the "purity" of the treatment during their production, that is, on the surface roughness.

The experiments were carried out at a MIG terawatt high-current generator with the current amplitude of up to 2.5 MA and its rise time of 100 ns. The load of the generator were cylindrical conductors made of stainless steel and steel 3 of the diameter 2 mm and length 15 mm. One half of the length (7.5 mm) at the cathode or anode side remained normal (after turning with a specified class of treatment equal to 6.3 with the largest size of inhomogeneities equal to 40 μm) and another half was treated additionally to increase or decrease the roughness of the surface. The experiments have shown that regardless of the surface roughness varying from units to hundreds of microns at a variable part of the load, the glow near the cathode part was always brighter and more uniform at the polished loads, but the difference in the time of the glow appearance (the 70-th ns) of both parts was less than the time of the camera exposure. That is, at the skin explosion, any noticeable influence of surface treatment on the time of the plasma formation onset was not observed with the conductors made of stainless steel and of stale 3.

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Skin electrical explosion of double-layer conductor with a low conductivity outer layer

Labetskaya N A[@], Datsko I M, Chaikovsky S A, Rybka D V and Shugurov V V

Institute of High Current Electronics of the Siberian Branch of the Russian Academy of Sciences, Akademichesky Avenue 2/3, Tomsk 634055, Russia

[@] natalia@ovpe2.hcei.tsc.ru

The plasma formation occurs on the electrodes surface in strong magnetic fields. That results in overlap of the vacuum gap by expanding plasma and deterioration of the transport efficiency of the energy to the generator load. In this paper the skin explosion of thick homogeneous and double-layer cylindrical conductors were studied at the threshold values of the magnetic field 200–400 T. Double-layer conductors were prepared by following technique. Titanium outer layer with low conductivity and thickness of 20–80 μm was deposited on the copper conductor by vacuum arc method on ion-plasma setup QUINTA. The experiments were carried out on the MIG high-current generator at a current level of up to 2.5 MA with a current rise time of 100 ns. It is shown that delay process of plasma formation higher 200 ns takes place at the use of double-layer structure conductor with a low conductivity outer layer compared with the homogeneous copper conductor. Calculations have shown that a delay of plasma formation can occur due to redistribution of the current density over the cross-section and reduce of the Joule heat on the surface of the double-layer conductor.

The effect of applied voltage frequency on surface dielectric barrier discharge plasma energy

Lazukin A V[1,@], Gundareva S V[1], Krivov S A[1], Nikitin A M[1], Kavyrshin D I[2] and Fedorovich S D[1]

[1] National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] lazukin_av@mail.ru

A surface dielectric barrier discharge (SDBD) is the basis for various electrical technologies. Whether an extended high-energy discharge with significant current or a low-energy low-temperature discharge can be obtained in unified electrode configuration for different purposes [1]. The results of experimental investigation of SDBD energy dependence on applied voltage frequency varying from 0.6 to 40 kHz in the axially symmetric planar electrode system are presented. For the first time it is determined that SDBD's plasma energy dependence on applied voltage frequency represents an U-shaped curve with a distinct minimum. Discharge energy decrease with frequency rise on a left part of the U-shaped curve is concerned with reduction of the cycle duration of plasma existence and therefore with reduction of the charging rate of the dielectric. After passing the minimum of the obtained U-shaped curve, thermal conductivities of the barrier and environment are found to be insufficient for complete heat dissipation with consequent temperature increase in the discharge area. Further rise of applied voltage frequency and a number of dielectric recharging lead to a rise of discharge energy. Increase of the dielectric barrier thermal conductivity prevents discharge transition to a leader form. SDBD's plasma energy dependence on applied voltage frequency on the aluminium nitride barrier has only decreasing character at least in the range of investigated frequencies.

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The ionization and deposition efficiency of substance, which simulates heavy components of a spent nuclear fuel (applied for plasma separation method of spent nuclear fuel)

Antonov N N[@], Samokhin A A, Zhabin S N, Val'yano G E, Gavrikov A V and Smirnov V P

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] antonovnickola@gmail.com

One needs a plasma sources of model substances to simulate experimentally the plasma separation method of spent nuclear fuel [1]. For this purpose, we carried out a kinetic and hydrodynamic simulation of the discharge with hot cathode in the lead vapor [2]. The simulation results showed that when discharge current density was near 3.5 A/cm^2 and the lead vapor concentration was near 2×10^{12} cm^{-3}, the ionization efficiency was close to 60%. We also carried out an experimental research of the discharge in the vapor lead with a hot cathode. For the creation of the vapor collection system we carried out research of the deposition coefficients of Pb on various substrates. The research results showed that deposition coefficients at medium temperatures of substrates near 70 °C did not drop lower than 75%.

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Ion mass separation in crossed electromagnetic fields as a part of the concept of spent nuclear fuel plasma separation

Gavrikov A V[1,2], Sidorov V S[1,@], Smirnov V P[1] and Tarakanov V P[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] vladimir.sidorov.89@gmail.com

Presented results have been obtained to develop the plasma separation study described in the article [1]. The main task is to calculate trajectories of ions of the substance imitating spent nuclear fuel in crossed electromagnetic fields. The calculations have been made with KARAT code in a single-particle approximation. The calculations have been performed for a number of combinations of azimuthal and axial magnetic fields and different electric fields configurations. Magnetic field is produced by 2–4 coils of wire, the characteristic field strength is up to 1.6 kG. Electric field is produced by 2–3 electrodes with electric potential up to 1 kV. The characteristic linear size of the calculation area is 100 cm. The characteristic size of injection region is 1 cm (up to 10 cm along main axis). Spatial position of the injection region and axis of the injection direction are varied. Injected particles are single-charged ions with energies from 0.2 to 3 eV with atomic masses $A = 150$ and 240, spreading angle is 60°. It is shown that there are several options to realize a spatial separation of spent nuclear fuel ions. Advantages and disadvantages from experimental point of view for each option are represented. The study was supported by grant from the Russian Science Foundation (project No. 14-29-00231).

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The parameters affecting the potential of the plasma column in the reflex discharge

Liziakin G D[1,@], Gavrikov A V[1,2], Usmanov R A[1,2] and Smirnov V P[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

[@] glizyakin@gmail.com

Currently there is little known about the establishment of a defined profile of the electric potential in the plasma. In the method of plasma separation [1] this is a key problem. While the end electrodes of the plasma separator is fed negative voltage, the vacuum chamber is grounded, which leads to the emergence of reflex discharge. This discharge generates a profile of the electric plasma potential. The work is devoted to the study of this profile.

In the paper reflex dc discharge in helium was explored. It was studied the effect of parameters such as magnetic field of 0.03 to 0.2 T, the pressure of 0.1–100 mTorr, discharge voltage of 0–1.2 kV, the distance cathode–cathode and cathode–anode on plasma column potential. It was shown that the dependence of the plasma column potential on pressure has two maxima. The position of the maxima was determined by the magnetic field. By isolated probe method was measured radial profile of the plasma potential. Using a double probe was measured concentration and the electron temperature. The range of the potential oscillations of the plasma column in different modes was defined.

The study was supported by a grant of the Russian Science Foundation (project No. 14-29-00231).

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Development of experimental setup for energy loss measurements in gas-discharge plasma on TIPr accelerator

Gavrilin R O[@], Rudskoi I V, Vysotsky S A, Golubev A A, Kuznetsov A P and Khabibullina E

State Scientific Center of the Russian Federation "Institute for Theoretical and Experimental Physics", National Research Center "Kurchatov Institute", Bolshaya Cheremushkinskaya 25, Moscow 117218, Russia

[@] roman_gavrilin@mail.ru

The measurement of the ion energy losses of in the ionized matter belongs to fundamental plasma physics, high energy density physics and inertial fusion with heavy ion beams research. The interaction of heavy ions with energy from 40 to 500 keV/nuclon and cold full-ionized plasma with lineal electron density near 10^{18} cm^{-2} is of interest within this problem. Over past few years a series of energy losses measurement experiments on linear accelerator in collaboration with Institute of Modern Physics (IMP CAS, Lanzhou, China) were made. Gas-discharge plasma target, produced [1] and diagnosed [2] in ITEP, was used in this experiments as plasma generator. Energy losses of projectile ions H^+, He^{1+}, He^{2+}, O^{4+}, O^{5+} with energies from 100 to 500 keV in cold gas and plasma were measured [3]. In addition, the two-wave laser interferometer for plasma target diagnostic was made in IMP by ITEP specialists. For further investigation, the new experimental setup in ITEP based on the TIPr linear accelerator will be created. It allows getting the experimental data of heavy ions with energies 100 keV/nuclon stopping power. For the energy-losses measurement, the time-of-flight method will be used.

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Spectral measurements of electron temperature of highly ionized He plasma in nonequilibrium conditions

Korshunov O V[1], Chinnov V F[1], Kavyrshin D I[1] and Ageev A G[2,@]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

[@] ageevalex@yandex.ru

It has been experimentally shown [1, 1] that highly ionized He arc plasma does not achieve local thermodynamic equilibrium expected for plasmas with electron concentrations above 1×10^{16} cm^{-3} [3, 4] like argon plasma [1]. We have found that the reason for this deviation is strong nonisotropy of plasma. The triple electron recombination with temperatures of 2.5–3 eV [1] is almost absent. The charged particles are moved from the arc ($r = 1$ mm [1]) onto chamber walls due to ambipolar diffusion creating ionization nonequilibrium over the excited states [4] rendering Boltzmann and Saha equations inapplicable for determining the electron temperature [3]. A method for determining electron temperature is suggested that is based on using the relative intensities of the atomic and ion lines. Its advantage lies in a energy gap between these lines' states over 50 eV that reduces the influence of nonequilibrium on the result. This influence can be taken into account if the ionization energies of emitting states of atom and ion have close values. The suggested method can be expanded for any media including those with dimensional nonisotropy having both atomic and ion lines in their emission spectra.

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Study of spatial distributions of highly ionized nonequilibrium helium plasma at atmospheric pressures

Chinnov V F[1], Kavyrshin D I[1,@], Ageev A G[2], Korshunov O V[1] and Sargsyan M A[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

[@] dimakav@rambler.ru

Experimental study of helium plasma at atmospheric pressure in the state of quasistationary heating was made. The plasma state is shown not to be described by Saha–Boltzmann approximation at high ionization levels $\alpha_i = 0.5$–0.9, temperatures of 2.5–4.0 eV and electron concentrations of about 1×10^{17} cm^{-3} [1]. The deviation from the equilibrium state of the plasma is caused by a lack of spatial uniformity due to charged particles loss by ambipolar diffusion. In order to thoroughly study the temporal changes of plasma radiation characteristics spectroscopic analysis was carried out with DFS-452 spectrometer and high-speed CMOS camera Andor iStar attached to its output. The system yields the spatial resolution of 30–50 μm and temporal resolution of 5–50 μs. Electron concentration n_e was measured from the half-width of the local HeI spectrum line contours displaying dominant quadruple Stark effect and having well-known constants [2, 3]. In order to determine the temperature of heavy particles, a triplet of HeI lines at 1083 nm Doppler component was studied. The temporal evolution of the following important characteristics has been determined for helium plasma during pulsed heating: current power, intensities of a number of HeI and HeII spectral lines, electron temperatures and concentrations.

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Features of spatial distribution of the parameters on the initial section of a supersonic plasma jet, created by pulsed discharge in a capillary with ablative wall

Pashchina A S, Efimov A V[@], Cninnov V F and Ageev A G

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] axletter@gmail.com

Pulse discharge in a capillary is used for creation a plasma jet. The capillary is fabricated from a carbon-containing polymer (polymethylmethacrylate, PMMA). Its initial diameter and depth are 1 and 4 mm, respectively. The design of the discharge gap, the experimental setup and methods of research are described in detail in [1]. Most researches of supersonic plasma jet are carried out for the following discharge pulse parameters: discharge pulse energy 80 J, the amplitude of the discharge current 400 A, the voltage drop across the discharge gap 200–250 V, the duration of the discharge pulse 1 ms, the peak discharge power 100 kW. Emission properties of high-temperature jet core (intensity and contour of Balmer lines H_α and H_β, the relative intensities of the ionic lines C_{II} and O_{II}) have been registered with high temporal (10 ms) and spatial (20–30 μm) resolution. It allowed us to reveal the main properties of pressure's space-time distribution, the temperature and the degree of ionization inside the capillary and heterogeneous supersonic jet. The presence of the molecular components exhibiting their emission properties at the plasma jet periphery permit us to estimate the parameters of the plasma in the spatial domain, where "detached" shock waves of the supersonic jet are created.

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The effect of gas bubbles on electrical breakdown in transformer oil

Sargsyan M A[@], Gadzhiev M Kh, Tyuftyaev A S, Akimov P L and Demirov N A

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] m.sargsyan86@mail.ru

Transformer oil is widely used as an insulator in various high-voltage machineries. Therefore the studies of discharge processes in oil filled high voltage apparatus where gas bubbles may be present initially or formed there by heating, electrolysis, cavitation etc. are of great interest. The dielectric strength of gases is much lower than dielectric strength of transformer oil and partial discharge may occur in the gas bubbles at the lower fields strengths than is necessary for a breakdown of oil. To investigate the breakdown of transformer oil and gas bubbles an experimental stand was constructed which included: a discharge chamber, a power source AI-70, voltage doubler, system of electrical, optical and spectral measurements [1,2]. It was found that the gassing of transformer oil by single gas bubbles reduces the breakdown voltage of oil. When the voltage between the electrodes is less than that necessary for the breakdown of the pure oil, the breakdown first occurs in the gas bubble and is not always overlapped by a highly conductive channel in the discharge gap. For example, the breakdown of the settled, used oil occurs at $V_{\rm av} = 85$ kV (distance between the electrodes—8mm). Gassing by single bubbles leads to a decrease in the breakdown voltage: ~ 60 kV—sulfur hexafluoride, 51 kV—air, 45 kV—argon, 37 kV—helium. Experimental results also showed that the repeated discharges in oil decrease the breakdown voltage due to the accumulation of oil decay products in the discharge gap. The work was supported by RSF grant No. 14-12-01295.

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Generator of chemically active low-temperature plasma

Sargsyan M A[@], Gadzhiev M Kh, Tyuftyaev A S, Demirov N A and Spector N O

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] m.sargsyan86@mail.ru

Generator of low-temperature plasma (GLP) has attracted the attention of specialists in the field of gas discharge physics and low-temperature plasma, and in the field of high-temperature gas dynamics by the fact that in the discharge gap of GLP the temperature range varies from thousands to tens of thousands degrees, which is of great interest for research in the thermal, electrical and optical properties of gases, as well as for research in various plasma-chemical reactions [1]. To study these parameters of chemically reactive plasma a generator of high enthalpy plasma jet was constructed with vortex stabilization and expanding anode channel. Dc plasma torch forms a slightly divergent ($2\alpha = 12^\circ$) nitrogen or air plasma jet with a diameter $D = 10$–12 mm with an enthalpy of 20–50 kJ/g (at total electric power of the arc discharge being 20–50 kW, plasma gas flow rate 1.0–2.0 g/s and the average weight temperature of the plasma at the outlet of 8–11 kK). The plasma chemical composition and the flow parameters of high-enthalpy plasma were determined by spectroscopic methods [1, 2]. The presence of atomic spectra of NI and OI in its respective plasmas allow to determine the electron temperature of plasma T_e. The concentration of electrons in the axial region of the plasma jet was estimated using the half-width of hydrogen atomic line H_α and H_β.

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Research methods of plasma stream interaction with heat-resistant materials

Sargsyan M A[1,@], Chinnov V F[1], Gadzhiev M Kh[1], Tyuftyaev A S[1], Demirov N A[1], Kavyrshin D I[1], Ageev A G[2] and Khromov M A[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

[@] m.sargsyan86@mail.ru

An experimental automated system was designed and constructed to study the parameters and characteristics of non-stationary interacting system "high enthalpy plasma stream–investigated sample": enthalpy of plasma in the incident stream; speed and temperature of plasma stream; temperature of electrons and heavy particles, ionic composition and their spatial distribution; heat flux incident on the sample (kW/cm^2); surface temperature of the sample; ablation of the sample material, and other. Measurements of achievable plasma heat flux levels are carried out by calorimetry of plasma streams incident on the surface of multi-section copper calorimeter. Determination of acceleration characteristics for profiled plasma torch nozzle, as well as the gas flow rate is produced by measuring the total pressure using the Pitot tube. Video visualization of interacting system is carried out using synchronized high-speed cameras. Micropyrometry of the selected zone on the sample surface is carried out by high-speed, three-wavelength pyrometer. To measure the rate of mass loss of the sample, in addition to the weighing method of evaluation the methods of "laser knife" and two-position stereoscopy are used. Plasma and sample emission characteristics are performed with two separate spectrometers. The work is supported by the Russian Ministry of Education as part of the Federal Program RFMEFI60414X0090.

AUTHOR INDEX

ORGANIZATION LIST

BMSTU — Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

BSTU — Belarusian State Technological University, Sverdlova Street 13a, Minsk 220006, Belarus

CIAM — Baranov Central Institute of Aviation Motors Development, Aviamotornaya Street 2, Moscow 111116, Russia

CSU — Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia

FIPCE RAS — Frumkin Institute of Physical Chemistry and Electrochemistry of the Russian Academy of Sciences, Leninsky Avenue 31, Moscow 199071, Russia

FiratUni — Firat University, Elazig 23169, Turkey

FSUE RFNC–VNIIEF — Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia

FSUE RFNC–VNIITF — Federal State Unitary Enterprise "Russian Federal Nuclear Center—Academician Zababakhin All-Russian Research Institute of Technical Physics", Vasilieva 13, Snezhinsk, Chelyabinsk Region 456770, Russia

GPI RAS — Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova 38, Moscow 119991, Russia

GSI — GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, Darmstadt 64291, Germany

HMTI NASB — Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus, P Brovka Street 15, Minsk 220072, Belarus

IAM RAS — Institute of Applied Mechanics of the Russian Academy of Sciences, Leninsky Avenue 32a, Moscow 117334, Russia

IAMA — Institute of Applied Mathematics and Automation, Shortanova 89a, Nalchik, Kabardino-Balkaria 360000, Russia

ICAD RAS — Institute for Computer-Aided Design of the Russian Academy of Sciences, Vtoraya Brestskaya 19/18, Moscow 123056, Russia

ICMM UB RAS — Institute of Continuous Media Mechanics of the Ural Branch of the Russian Academy of Sciences, Academician

Korolev Street 1, Perm 614013, Russia

ICP RAS — Semenov Institute of Chemical Physics of the Russian Academy of Sciences, Kosygina 4, Moscow 119991, Russia

IEE RAS — Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, Russia

IEP UB RAS — Institute of Electrophysics of the Ural Branch of the Russian Academy of Sciences, Amundsen 106, Ekaterinburg 620016, Russia

IGM SB RAS — Sobolev Institute of Geology and Mineralogy of the Siberian Branch of the Russian Academy of Sciences, Akademika Koptyuga 3, Novosibirsk 630090, Russia

IGR DSC RAS — Institute for Geothermal Research of the Daghestan Scientific Center of the Russian Academy of Sciences, Shamil 39a, Makhachkala, Daghestan 367030, Russia

IHCE SB RAS — Institute of High Current Electronics of the Siberian Branch of the Russian Academy of Sciences, Akademichesky Avenue 2/3, Tomsk 634055, Russia

IIC SB RAS — Institute of Inorganic Chemistry of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 3, Novosibirsk 630090, Russia

IKI RAS — Space Research Institute of the Russian Academy of Sciences, Profsoyuznaya 84/32, Moscow 117997, Russia

INEPCP RAS — Institute of Energy Problems of Chemical Physics of the Russian Academy of Sciences, Leninsky Avenue 38 Corps 2, Moscow 117829, Russia

IngGU — Ingush State University, Magistralnaya 39, Nazran, Ingushetia 386001, Russia

IPCP RAS — Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

IPME RAS — Institute of Problems of Mechanical Engineering of the Russian Academy of Sciences, V.O., Bolshoj pr., 61, Saint Petersburg 199178, Russia

ISA RAS — Institute for Systems Analysis of the Russian Academy of Sciences, 60-letiya Oktyabrya 9, Moscow 117312, Russia

ISPMS SB RAS — Institute of Strength Physics and Material Science of the Siberian Branch of the Russian Academy of Sciences, Akademicheskii 2/4, Tomsk 634021, Russia

ISSP RAS — Institute of Solid State Physics of the Russian Academy of Sciences, Institutskaya Street 2, Chernogolovka, Moscow Region 142432, Russia

ITAM SB RAS — Institute of Theoretical and Applied Mechanics of the Siberian Branch of the Russian Academy of Sciences, Institutskaya 4/1, Novosibirsk 630090, Russia

ITNE — Institute for Time Nature Exploration of the Moscow State University, Faculty of Biology, Division of General Ecology, Leninskiye Gory 1-12, Moscow 119991, Russia

ITP RAS — Landau Institute for Theoretical Physics of the Russian Academy of Scienses, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia

ITP UB RAS — Institute of Thermophysics of the Ural Branch of the Russian Academy of Sciences, Amundsen Street 107a, Ekaterinburg 620016, Russia

JIHT RAS — Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

KAUST — King Abdullah University of Science and Technology, 4-2226, 4700 KAUST, Thuwal, Makkah 23955, Saudi Arabia

KAZNU — Al-Farabi Kazakh National University, al-Farabi Avenue 71, Almaty 050040, Kazakhstan

KAZNU, IETP — Research Institute of Experimental and Theoretical Physics of the Al-Farabi Kazakh National University, al-Farabi Avenue 71, Almaty 050040, Kazakhstan

KBSC RAS — Kabardino-Balkarian Scientific Center of the Russian Academy of Sciences, Inessa Armand 37, Nalchik, Kabardino-Balkaria 360051, Russia

KBSU — Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia

KFU — Kazan Federal University, Kremlyovskaya 18, Kazan, Tatarstan 420008, Russia

KIAM RAS — Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, Miusskaya Square 4, Moscow 125047, Russia

KubSTU NPI — Novorossiysk Polytechnic Institute of the Kuban State Technical University, Karl Marx 20, Novorossiysk 353900, Russia

LIH SB RAS — Lavrentyev Institute of Hydrodynamics of the

Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 15, Novosibirsk 630090, Russia

LPDS TMBU — Laboratory of Semiconductor Device Physics of the Tahri Mohamed Bechar University, P.O.B. n°417, Bechar 08000, Algeria

LPI RAS — Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

MA SRT — Military Academy of Strategic Rocket Troops after Peter the Great, Kitaygorodskiy 9, Moscow 109074, Russia

MAI — Moscow Aviation Institute, Volokolamskoe Shosse 4, Moscow 125993, Russia

Makeyev GRTs — Open Joint Stock Company "Academician Makeyev State Rocket Centre", Turgoyakskoye Shosse 1, Miass, Chelyabinsk Region 456300, Russia

MIEM HSE — Moscow Institute of Electronics and Mathematics, National Research University Higher School of Economics, Tallinskaya 34, Moscow 123458, Russia

MIPT — Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

NRC KI — National Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia

NRNU MEPhI — National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

NRU MPEI — National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

NSU — Novosibirsk State University, Pirogova Street 2, Novosibirsk 630090, Russia

OGRI RAS — Oil and Gas Research Institute of the Russian Academy of Sciences, Gubkin Street 3, Moscow 119991, Russia

PSU — Perm State University, Bukireva Street 15, Perm 674990, Russia

RDB named after A.Lyulka — Research and Design Bureau named after A Lyulka, Kasatkin Street 13, Moscow 129301, Russia

RRC KI, INS — Institute of Nuclear Synthesis of the Russian Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia

RSAU–TMAA — Russian State Agrarian University—Timiryazev

Moscow Agricultural Academy, Timiryazevskaya 49, Moscow 127550, Russia

SMR — Schlumberger Moscow Research Center, Pudovkina 13, Moscow 119285, Russia

SPbPU — Peter the Great Saint-Petersburg Polytechnic University, Polytechnicheskaya 29, Saint-Petersburg 195251, Russia

SPbSU ITMO — Saint-Petersburg State University of Information Technologies, Mechahics and Optics, Kronvergskiy 49, Saint-Petersburg 197101, Russia

SRC RF TRINITI — State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 142190, Russia

SSC RF IPPE — Joint Stock Company "State Scientific Centre of the Russian Federation—Institute for Physics and Power Engineering named after A I Leypunsky", Bondarenko Square 1, Obninsk, Kaluga Region 249033, Russia

SSC RF ITEP — State Scientific Center of the Russian Federation "Institute for Theoretical and Experimental Physics", National Research Center "Kurchatov Institute", Bolshaya Cheremushkinskaya 25, Moscow 117218, Russia

STC "Industrial Safety Research" — Scientific and Technical Centre "Industrial Safety Research", Perevedenovsky 13 Bldg 14, Moscow 105082, Russia

Streamer Inc. — Streamer, Electric Company Inc., Office 17N, Nevsky Prospect 147, Saint-Petersburg 191024, Russia

SUSU — South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia

TSTU — Tambov State Technical University, Sovetskaya Street 106, Tambov 392000, Russia

TSU, RIAMM — Research Institute of Applied Mathematics and Mechanics of the Tomsk State University, Lenin Avenue 36, Tomsk 634050, Russia

TSUAB — Tomsk State University of Architecture and Building, Solyanaya Square 2 Bldg 2, Tomsk 634003, Russia

TUBAF — Technical University Bergakademie Freiberg, Freiberg, Germany

UrFU — Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

VNIIA(L) — All-Russia Research Institute of Automatics named

after Dukhov, Luganskaya 9, Moscow 115304, Russia

VNIIA(S) — All-Russia Research Institute of Automatics named after Dukhov, Sushchevskaya 22, Moscow 127055, Russia

WCRC — Western-Caucasus Research Center, Tupik Zvezdniy 9, Tuapse, Krasnodar Territory 352808, Russia

PARTICIPANT LIST

1. *Abramov Maxim Alexandrovich*, CIAM, abramovmaks94@gmail.com
2. *Adiguzel Osman*, FiratUni, +90(424)2370000, oadiguzel@hotmail.com
3. *Ageev Aleksey Gennadievich*, NRU MPEI, ageevalex@yandex.ru
4. *Akhmatov Zeitun Anuarovich*, KBSU, +7(866)2775111, ahmatov.z@bk.ru
5. *Akzyanov Ramil Sharifullovich*, VNIIA(L), apexgreen57@gmail.com
6. *Alkhimova Mariya Andreevna*, JIHT RAS, MAAlkhimova@mephi.ru
7. *Amirov Ravil Khabibulovich*, JIHT RAS, +7(495)4859777, mshavelkina@gmail.com
8. *Anan'ev Sergei Yurevich*, JIHT RAS, serg.ananev@gmail.com
9. *Ananyan Marlen Valerievich*, CIAM, marlen@ciam.ru
10. *Andreev Nikolay Evgen'evich*, JIHT RAS, +7(495)4859722, andreev@ras.ru
11. *Andryushin Ivan*, SSC RF IPPE, i.andryushin@gmail.com
12. *Antonov Nikolay Nikolaevich*, JIHT RAS, antonovnickola@gmail.com
13. *Apfelbaum Evgeny Mikhailovich*, JIHT RAS, +7(495)4844433, apfel_e@mail.ru
14. *Arefyev Konstantin Yuryevich*, CIAM, arefyev@ciam.ru
15. *Ashitkov Sergey Igorevich*, JIHT RAS, +7(495)2294240, ashitkov11@yandex.ru
16. *Atroshenko Svetlana Alekseevna*, IPME RAS, +7(812)3214765, satroshe@mail.ru
17. *Avdeeva Anna Vyacheslavovna*, CSU, awdeewaanya@yandex.ru
18. *Avdonin Vladimir Vladimirovich*, IPCP RAS, +7(496)5221756, shakhray@icp.ac.ru
19. *Azeddine Bouziane*, LPDS TMBU, +213(06)60076822, bouziane60@mail.ru
20. *Babaeva Natalia Yuryevna*, JIHT RAS, nybabaeva@gmail.com

21. *Baidakov Vladimir Georgievich*, ITP UB RAS, +7(343)2678801, baidakov@itp.uran.ru
22. *Bannikova Irina Anatolevna*, ICMM UB RAS, +7(342)2378312, malgacheva@mail.ru
23. *Bardin Andrey Alex*, IPCP RAS, dr.abardin@gmail.com
24. *Barenbaum Azary Aleksandrovich*, OGRI RAS, +7(499)1357221, azary@mail.ru
25. *Barengolts Sergey Aleksandrovich*, GPI RAS, sabarengolts@mail.ru
26. *Baronova Elena Olegovna*, RRC KI, INS, +7(499)1967703, baronova04@mail.ru
27. *Basharin Andrey Yurievich*, JIHT RAS, +7(495)3625603, abasharin@bk.ru
28. *Batuev Stanislav*, TSUAB, spbatuev@gmail.com
29. *Batura Stanislav Nikolaevich*, CIAM, since85@mail.ru
30. *Bayandin Yuriy Vitalievich*, ICMM UB RAS, +7(342)2378312, buv@icmm.ru
31. *Belikov Roman Sergeyevich*, JIHT RAS, ihatepesh@mail.ru
32. *Belkheeva Rumiya Katdusovna*, NSU, rumia@post.nsu.ru
33. *Bivol Grigory Yurievich*, JIHT RAS, +7(495)4858463, grigorij-bivol@yandex.ru
34. *Bobrov Andrei Alexandrovich*, JIHT RAS, abobrov@inbox.ru
35. *Bobrov Victor Borisovich*, JIHT RAS, vic5907@mail.ru
36. *Bocharnikov Vladimir Maksimovich*, JIHT RAS, vova.m.bocha@gmail.com
37. *Bocharov Aleksey Nikolaevich*, JIHT RAS, +7(495)4842638, bocharov@ihed.ras.ru
38. *Bogdanov Anton Valentinovich*, SSC RF ITEP, toshka87@list.ru
39. *Bogdanova Youlia Andreevna*, NRNU MEPhI, bogdanova.youlia@bk.ru
40. *Bogomaz Alexander Alexeevich*, IEE RAS, +7(812)3151757, bogomazal@rambler.ru
41. *Bolesta Alexey Vladimirovich*, ITAM SB RAS, +7(383)3303804, bolesta@itam.nsc.ru
42. *Boriev Igor Abuzedovich*, INEPCP RAS, +7(496)5223349, boriev@binep.ac.ru
43. *Borodin Elijah Nikolaevich*, IPME RAS, elbor7@gmail.com
44. *Brovkin Vadim Gennadievich*, JIHT RAS, brovkin47@mail.ru

45. *Bryuzgin Svyatoslav Valerievich*, JIHT RAS, nikel.26@mail.ru
46. *Bugay Irina Vladimirovna*, IAM RAS, ibug@mail.ru
47. *Butlitsky Michael Anatolyevich*, JIHT RAS, aristofun@yandex.ru
48. *Buzyurkin Andrey Evgenievich*, ITAM SB RAS, buzjura@itam.nsc.ru
49. *Bystryi Roman*, JIHT RAS, broman.meld@gmail.com
50. *Chernik Marina Yur'evna*, HMTI NASB, +375(29)2275213, Emerald_@tut.by
51. *Chigvintsev Alexander*, MIPT, alex012008@gmail.com
52. *Chingina Evgeniya Andreevna*, IEP UB RAS, +7(343)2678776, zhenya@iep.uran.ru
53. *Chinnov Valeriy Fedorovich*, JIHT RAS, v_chinnov@oivtran.ru
54. *Chusov Alexander Nikolaevich*, Streamer Inc., chusov86@gmail.com
55. *Danilov Mikhail Konstantinovich*, CIAM, danilovm@ciam.ru
56. *Datsko Igor Mikhailovich*, IHCE SB RAS, +7(382)2491677, datsko@ovpe.hcei.tsc.ru
57. *Degtayrev Andrey Aleksandrovich*, FSUE RFNC–VNIITF, a.a.degtjarjov@gmail.com
58. *Degtiar Vladimir Grigoryevich*, Makeyev GRTs, +7(3513)286370, src@makeyev.ru
59. *Degtyareva Valentina Feognievna*, ISSP RAS, +7(486)5228376, degtyar@issp.ac.ru
60. *Director Leonid Bentsianovich*, JIHT RAS, +7(495)4859144, director@oivtran.ru
61. *Dolnikov Gennady Gennadjevich*, IKI RAS, +7(495)3332566, ggd@iki.rssi.ru
62. *Doludenko Aleksey Nikolaevich*, JIHT RAS, +7(495)4859666, adoludenko@gmail.com
63. *Dozhdikov Vitaly Stanislavovich*, JIHT RAS, +7(495)3625603, vdozh@mail.ru
64. *Dyachkov Lev Gavriilovich*, JIHT RAS, +7(495)3625310, dyachk@mail.ru
65. *Dyachkov Sergey Aleksandrovich*, VNIIA(L), serj.dyachkov@gmail.com
66. *Ebel Andrej Alexandrovich*, SUSU, ebel_aa@rambler.ru
67. *Efimchenko Vadim Sergeevich*, ISSP RAS, +7(496)5228410,

efimchen@issp.ac.ru
68. *Efimov Alexander Valerevich*, JIHT RAS, axletter@gmail.com
69. *Efremov Vladimir Petrovich*, JIHT RAS, +7(495)4850963, dr.efremov@gmail.com
70. *Egorov Oleg Georgievich*, SRC RF TRINITI, +7(498)5405058, egorov@triniti.ru
71. *Egorova Maria Sergeevna*, VNIIA(S), egorova.maria.serg@gmail.com
72. *Emelianov Alexander Valentinovich*, JIHT RAS, +7(495)4841966, aemelia@ihed.ras.ru
73. *Emelin Dmitriy Anatolyevich*, SUSU, emelin_d_a@mail.ru
74. *Emelyanov Andrey Nikolaevich*, IPCP RAS, +7(496)5221766, emelyanov@ficp.ac.ru
75. *Eremin Alexander Victorovich*, JIHT RAS, +7(495)4832314, eremin@ihed.ras.ru
76. *Erenburg Simon Borisovich*, IIC SB RAS, +7(383)3304447, simon@niic.nsc.ru
77. *Evstigneev Nikolay Mikhaylovitch*, ISA RAS, evstigneevnm@yandex.ru
78. *Fedotova Ksenya Victorovna*, CIAM, wonnahrefn@icloud.com
79. *Fidanyan Karen Sarkisovich*, JIHT RAS, karencho616@yandex.ru
80. *Filinov Vladimir Sergeevich*, JIHT RAS, +7(495)4842429, vladimir_filinov@mail.ru
81. *Filippov Anatoly Vasilievich*, SRC RF TRINITI, +7(495)8415262, fav@triniti.ru
82. *Filippov Evgeny Dmitrievich*, JIHT RAS, nopers@bk.ru
83. *Fokin Vladimir Borisovich*, JIHT RAS, +7(495)4842456, Vladimir.fokin@phystech.edu
84. *Fortov Vladimir Evgenievich*, JIHT RAS, +7(495)4857988, fortov@ihed.ras.ru
85. *Fortova Svetlana Vladimirovna*, ICAD RAS, sfortova@mail.ru
86. *Frantsuzov Maxim Sergeevich*, CIAM, mfrancuzov@yandex.ru
87. *Frolov Alexander Anatol'evich*, JIHT RAS, +7(495)4859722, frolov@ihed.ras.ru
88. *Gabderakhmanova Tatiana Sergeevna*, JIHT RAS, tts_91@mail.ru
89. *Gadzhiev Makhach Khairudinovich*, JIHT RAS, makhach@mail.ru

90. *Galitskaya Yelena Alexanrovna*, ISSP RAS, +7(496)5228410, galitskaya@issp.ac.ru
91. *Galiullina Gulnaz Maratovna*, JIHT RAS, gulnaz_g@inbox.ru
92. *Garkushin Gennady*, IPCP RAS, +7(496)5249472, garkushin@ficp.ac.ru
93. *Gavasheli Yuliya Olegovna*, KBSU, yu-pakhunova@mail.ru
94. *Gavrikov Andrey Igorevich*, NRC KI, +7(499)1967706, Gavrikov_AI@nrcki.ru
95. *Gavrilin Roman*, SSC RF ITEP, roman_gavrilin@mail.ru
96. *Golovastov Sergey*, JIHT RAS, golovastov@yandex.ru
97. *Golub Victor Vladimirovich*, JIHT RAS, +7(495)4842138, victor.v.golub@gmail.com
98. *Golubev Alexander Alexandrovich*, SSC RF ITEP, +7(499)1274735, golubev@itep.ru
99. *Golyshev Andrey Anatolievich*, IPCP RAS, +7(496)5227225, golyshev@icp.ac.ru
100. *Gribov Iourii Aronovich*, ITNE, +7(499)7264769, jgribov@yandex.ru
101. *Gubskiy Konstantin Leonidovich*, NRNU MEPhI, kgubskiy@mail.ru
102. *Gurtovoy Sergey Antonovich*, JIHT RAS, skrafy@bk.ru
103. *Ignatov Alexander Mikhailovich*, GPI RAS, aign@fpl.gpi.ru
104. *Ilnitskiy Denis*, VNIIA(L), denisilnitskiy@gmail.com
105. *Inogamov Nail*, ITP RAS, +7(495)7029317, nailinogamov@gmail.com
106. *Iosilevskiy Igor L'vovich*, JIHT RAS, Iosilevskiy@gmail.com
107. *Is'yomin Rafail Lvovich*, TSTU, +7(4752)630446, risemin@gmail.com
108. *Ismagambetova Tomiris*, KAZNU, +7(727)3773174, miriael@mail.ru
109. *Ivanin Oleg Alexandrovich*, JIHT RAS, oleggin2006@yandex.ru
110. *Ivanov Mikhail Fedorovich*, JIHT RAS, +7(495)4844433, ivanov_mf@mail.ru
111. *Ivanov Mikhail Ivanovich*, VNIIA(S), ivanov3575@yandex.ru
112. *Izvekov Oleg Yaroslavovich*, MIPT, +7(495)4084827, izvekov_o@inbox.ru
113. *Kachalov Vladimir Victorovich*, JIHT RAS, +7(495)4859145, ongk@mail.ru

114. *Kadatskiy Maxim Alekseevich*, JIHT RAS, Makkad@yandex.ru
115. *Kalashnikov Sergey Timofeyevich*, Makeyev GRTs, +7(3513)286370, src@makeyev.ru
116. *Kanel Gennady Isaakovich*, JIHT RAS, +7(495)4834374, kanel@ficp.ac.ru
117. *Karpyshev Pavel Aleksandrovich*, JIHT RAS, pavel.karpyshev@phystech.edu
118. *Kashkarov Alexey Olegovich*, LIH SB RAS, kashkarov@hydro.nsc.ru
119. *Kasimov Aslan*, KAUST, +9(665)44700076, aslankasimov@gmail.com
120. *Kaunov Victor Sergeevich*, KubSTU NPI, nvr10@mail.ru
121. *Kavyrshin Dmitry Igorevich*, JIHT RAS, +7(495)4841855, dimakav@rambler.ru
122. *Kazakov Evgeny Davidovich*, NRC KI, evgenische@gmail.com
123. *Kazanskiy Pavel Nikolaevich*, JIHT RAS, fokkoo@yandex.ru
124. *Khirianova Alexandra Igorevna*, MIPT, khirianova.alexandra@gmail.com
125. *Khishchenko Konstantin Vladimirovich*, JIHT RAS, +7(495)4842483, konst@ihed.ras.ru
126. *Khlybov Vladimir Ilyich*, Makeyev GRTs, vik_20152016@mail.ru
127. *Khlyupin Aleksey Nikolaevich*, SMR, khlyupin@phystech.edu
128. *Khokhlov Victor Alexandrovich*, ITP RAS, khokhlov@landau.ac.ru
129. *Khokonov Azamat Khazret-Alievich*, KBSU, +7(866)2775111, azkh@mail.ru
130. *Khokonov Murat Khazretalievich*, KBSU, khokon6@mail.ru
131. *Khromova Elena Sergeevna*, IPCP RAS, +7(49652)24471, khromova@icp.ac.ru
132. *Kirova Elena Mikhailovna*, JIHT RAS, kirova@phystech.edu
133. *Kislenko Sergey Aleksandrovich*, JIHT RAS, kislenko@ihed.ras.ru
134. *Kiverin Alexey*, JIHT RAS, +7(495)4844433, alexeykiverin@gmail.com
135. *Klementyeva Irina*, JIHT RAS, ira.klementyeva@mail.ru
136. *Klyuchenovich Ekaterina Alexandrovna*, JIHT RAS, +7(495)4858354, zabelinakatia@mail.ru

137. *Knyazev Dmitry Vladimirovich*, JIHT RAS, +7(495)4842456, d.v.knyazev@yandex.ru
138. *Kochetkova Nina Sergeevna*, IPCP RAS, +7(49652)49472, gns@ficp.ac.ru
139. *Kochurin Evgeny Aleksandrovich*, IEP UB RAS, kochurin@iep.uran.ru
140. *Kolesnikov Dmitry Sergeevich*, SSC RF ITEP, dstorm1@mail.ru
141. *Kolesnikova Maria Alekseevna*, MIPT, pestovsky@phystech.edu
142. *Kolotova Lada Nikolaevna*, JIHT RAS, +7(495)4858545, lada.kolotova@gmail.com
143. *Kondratyev Arseniy Mikhailovich*, JIHT RAS, cpl593h@mail.ru
144. *Kondratyuk Nickolay Dmitrivich*, JIHT RAS, kondratyuk@phystech.edu
145. *Konyukhov Andrey Victorovich*, JIHT RAS, +7(495)5908620, konyukhov_av@mail.ru
146. *Korneva Maria Andreevna*, JIHT RAS, marijakorneva@yandex.ru
147. *Korobov Andrey Evgenevich*, JIHT RAS, +7(495)4858463, andrusha.kor@gmail.com
148. *Korotaev Pavel Yurievich*, VNIIA(S), korotaev@vniia.ru
149. *Koshkin Dmitrii Sergeevich*, NRNU MEPhI, l33dpr0g0x55@gmail.com
150. *Kosov Valentin Vladimirovich*, JIHT RAS, +7(495)4858354, kosov@ihed.ras.ru
151. *Koss Xeniya Georgievna*, JIHT RAS, +7(495)4842355, Xeniya.Koss@gmail.com
152. *Kostenko Oleg Fedotovich*, JIHT RAS, +7(495)4859722, olegkost@ihed.ras.ru
153. *Kozerod Aleksandr Vladimirovich*, CIAM, kozerod@me.com
154. *Kozlov Aleksey Aleksandrovich*, JIHT RAS, alexk5577@yandex.ru
155. *Krasnikov Vasiliy*, CSU, vas.krasnikov@gmail.com
156. *Krasnova Polina Andreevna*, JIHT RAS, +7(495)4842456, pakrasnova@gmail.com
157. *Krasyuk Igor Kornelievich*, GPI RAS, +7(499)5038130, krasyuk99@rambler.ru

158. *Kraus Evgeny Ivanovich*, ITAM SB RAS, +7(383)3303880, kraus@itam.nsc.ru
159. *Kravchenko Igor Vitalievich*, IPCP RAS, krav@ficp.ac.ru
160. *Krikunova Anastasia Igorevna*, JIHT RAS, utro-2007@mail.ru
161. *Krivosheev Sergey Ivanovich*, SPbPU, ksi.mgd@rambler.ru
162. *Kudryavtsev Dmitriy Aleksandrovich*, SPbSU ITMO, +7(812)3147864, togg1@yandex.ru
163. *Kudryavtseva Irina Vladimirovna*, SPbSU ITMO, +7(812)3147864, togg1@yandex.ru
164. *Kukshinov Nikolay Vladimirovich*, CIAM, kukshinov@ciam.ru
165. *Kulikov Yury Matveevich*, JIHT RAS, kulikov-yurii@yandex.ru
166. *Kurilenkov Yuri Konstantinovich*, JIHT RAS, +7(495)4841647, kurilenkovyuri@gmail.com
167. *Kurochka Kirill Victorovich*, UrFU, kirill.k.v@yandex.ru
168. *Kuzmina Julia Sergeevna*, JIHT RAS, juli_kuzmina@mail.ru
169. *Kuznetsov Andrey Petrovich*, NRNU MEPhI, apkuznetsov@mephi.ru
170. *Kuznetsov Sergey Vyacheslavovich*, JIHT RAS, +7(495)4859722, shenau@rambler.ru
171. *Kyarov Aslan Khasanovich*, KBSU, +7(8662)423777, ktf@kbsu.ru
172. *Labetskaya Natalia Anatolievna*, IHCE SB RAS, +7(3822)492133, natalia@ovpe2.hcei.tsc.ru
173. *Lankin Alexander Valerievich*, JIHT RAS, Alex198508@yandex.ru
174. *Lapitsky Dmitry Sergeevich*, JIHT RAS, +7(495)4842429, dmitrucho@yandex.ru
175. *Larina Olga Mikhailovna*, JIHT RAS, +7(495)4842447, umnova.olya@gmail.com
176. *Latypov Fanil*, CSU, latypovfanil@gmail.com
177. *Lavrenov Vladimir Alexandrovich*, JIHT RAS, v.a.lavrenov@gmail.com
178. *Lavrinenko Yaroslav Sergeevich*, JIHT RAS, lavrinenko@phystech.edu
179. *Lazukin Alexander Vadimovich*, NRU MPEI, lazukin_av@mail.ru
180. *Lebedeva Marina Yur'evna*, IPCP RAS, +7(49652)49472, marina@ficp.ac.ru

181. *Lenev Dmitrii Yurievich*, JIHT RAS, lenevdy@mail.ru
182. *Lepeshkin Alexander Roaldovich*, CIAM, +7(495)5529634, lepeshkin.ar@gmail.com
183. *Leschevich Vladimir Vladimirovich*, HMTI NASB, +375(17)2841520, v.leschevich@dnp.itmo.by
184. *Lesnikova Darya Sergeevna*, PSU, dslesnikova@gmail.com
185. *Levashov Pavel Remirovich*, JIHT RAS, +7(495)4842456, pasha@ihed.ras.ru
186. *Likhachev Alexandr Pavlovich*, JIHT RAS, +7(495)4842338, apl@ihed.ras.ru
187. *Lisanov Michail Viacheslavovich*, STC "Industrial Safety Research", +7(495)6204750, sumskoi@mail.ru
188. *Lisin Evgeny*, JIHT RAS, +7(495)4842355, eaLisin@yandex.ru
189. *Lisina Irina Igorevna*, JIHT RAS, +7(495)4842355, Irina.Lisina@mail.ru
190. *Liziakin Gennadii Dmitrievich*, JIHT RAS, glizyakin@gmail.com
191. *Loktionov Egor Yuryevitch*, BMSTU, +7(499)2636299, stcpe@bmstu.ru
192. *Lomonosov Igor Vladimirovich*, IPCP RAS, +7(496)5224124, ivl143@yandex.ru
193. *Lopanitsyna Nataliya Yurievna*, JIHT RAS, +7(495)4858545, lopanitsyna@phystech.edu
194. *Lukin Alexander Nickolaiyevitch*, WCRC, lukin@wcrc.ru
195. *Lunev Artem Vladimirovitch*, JIHT RAS, AVLunev@mephi.ru
196. *Maevskii Konstantin Konstantinovich*, LIH SB RAS, +7(383)3331891, konstantinm@hydro.nsc.ru
197. *Magomedov Ramazan Abdullaevich*, IGR DSC RAS, ramazan_magomedov@rambler.ru
198. *Maiorov Sergey Alekseevich*, GPI RAS, +7(499)1350247, mayorov_sa@mail.ru
199. *Makarov Sergey Stanislavovich*, JIHT RAS, seomakarov28@gmail.com
200. *Makhnach Anastasiya*, HMTI NASB, +7(529)6202099, mahnach_anna@mail.ru
201. *Maltsev Maxim Alexandrovich*, JIHT RAS, daerus21@yandex.ru

202. *Manykin Eduard Anatolievich*, NRC KI, edman17@mail.ru
203. *Markova Tatiana Valerievna*, JIHT RAS, markova@flowvision.ru
204. *Martynova Inna Aleksandrovna*, JIHT RAS, martina1204@yandex.ru
205. *Matveeva Natalia Andreevna*, JIHT RAS, nataliematveeva1@gmail.com
206. *Mayer Alexander Evgenievich*, CSU, mayer@csu.ru
207. *Medvedev Sergey Pavlovich*, ICP RAS, +7(495)9397302, s_p_medvedev@chph.ras.ru
208. *Melnikova Nina Vladimirovna*, UrFU, nvm.melnikova@gmail.com
209. *Mendeleyev Vladimir Yakovlevich*, JIHT RAS, +7(495)4859727, v_mendeleyev@ihed.ras.ru
210. *Merkulov Evgeniy Sergeevich*, Makeyev GRTs, mes1@yandex.ru
211. *Mesyats Vadim Gennadevich*, GPI RAS, sabarengolts@mail.ru
212. *Migdal Kirill Petrovich*, VNIIA(S), +7(499)9728413, migdal@vniia.ru
213. *Mikhaylyuk Andrey Vladimirovich*, NRNU MEPhI, andrey1990_mephi@mail.ru
214. *Mikushkin Anton Yuryevich*, JIHT RAS, mikushkin-anton@yandex.ru
215. *Minakov Dmitry*, JIHT RAS, minakovd@ihed.ras.ru
216. *Mintsev Victor Borisovich*, IPCP RAS, +7(49652)24475, minvb@icp.ac.ru
217. *Mochalova Valentina*, IPCP RAS, +7(49652)24125, roxete20000@hotmail.com
218. *Molchanov Dmitry Anatolyevich*, JIHT RAS, dmitriy.molchanov13@gmail.com
219. *Moldabekov Zhandos*, KAZNU, IETP, +7(778)2179543, zhandos@physics.kz
220. *Molodets Alexander Mikhailovich*, IPCP RAS, +7(49652)21049, molodets@icp.ac.ru
221. *Moseev Dmitry Sergeevich*, CIAM, dmitmoseev@yandex.ru
222. *Munhoz Daniel da Silva*, JIHT RAS, dasmunhoz@yahoo.com.br
223. *Murashkin Dmitry Andreevich*, JIHT RAS, 3995@mail.ru

224. *Murzov Semen Alexandrovich*, VNIIA(S), semen.murzov@phystech.edu
225. *Musikhin Stanislav Alexeevich*, JIHT RAS, stasntsk@gmail.com
226. *Myasnikov Maxim*, JIHT RAS, miasnikovmi@mail.ru
227. *Narkevich Ivan Ivanovich*, BSTU, +375(17)3994960, inarkevich@mail.ru
228. *Nesterenko Alexey Olegovich*, VNIIA(S), radamat@rambler.ru
229. *Nikolaev Alexey Yurievich*, FSUE RFNC–VNIITF, alexeyrx350@yandex.ru
230. *Nikolaev Dmitry Nikolaevich*, IPCP RAS, nik@ficp.ac.ru
231. *Nikolaev Vladislav Sergeevich*, JIHT RAS, vladiorussia@mail.ru
232. *Noginova Ludmila*, RSAU–TMAA, ludmilaun7@mail.ru
233. *Norman Genri Edgarovich*, JIHT RAS, +7(495)4858545, genri.norman@gmail.com
234. *Obruchkova Liliya Rimovna*, JIHT RAS, +7(495)4850963, o_liliya@ihed.ras.ru
235. *Ochkov Valery Fedorovich*, NRU MPEI, +7(495)3627171, evgust@gmail.com
236. *Oginov Alexander Vladimirovich*, LPI RAS, +7(499)1326468, oginov@lebedev.ru
237. *Oleynikova Elena Nikolaevna*, JIHT RAS, +7(495)4858536, oleynikova-en@mail.ru
238. *Orekhov Maksim Aleksandrovich*, JIHT RAS, mo2411@mail.ru
239. *Orekhov Nikita*, JIHT RAS, nikita.orekhov@gmail.com
240. *Oreshkin Evgeny Vladimirovich*, LPI RAS, +7(499)1326614, oreshkin@lebedev.ru
241. *Oreshkin Vladimir Ivanovich*, IHCE SB RAS, +7(3822)492988, oreshkin@ovpe.hcei.tsc.ru
242. *Orlov Maxim Yurevich*, TSU, RIAMM, +7(3822)529569, orloff_m@mail.ru
243. *Orlov Nikolay Yurievich*, JIHT RAS, +7(495)4842456, nyuorlov@mail.ru
244. *Ostrik Afanasy Victorovich*, IPCP RAS, ostrik@ficp.ac.ru
245. *Panchenko Alexei Nicolaevich*, IHCE SB RAS, +7(3822)492392, alexei@loi.hcei.tsc.ru

246. *Panov Vladislav Alexandrovich*, JIHT RAS, panovvladislav@gmail.com
247. *Patlazhan Stanislav*, IPCP RAS, sapat@yandex.ru
248. *Pavlov Sergey Vladimirovich*, JIHT RAS, sergey.v.pavlov@phystech.edu
249. *Pazyuk Yulia*, JIHT RAS, tightcookie@mail.ru
250. *Pecherkin Vladimir Yakovlevich*, JIHT RAS, +7(495)4841810, vpecherkin@yandex.ru
251. *Pesochin Vladimir Romanovich*, JIHT RAS, +7(495)4842429, syrovatkara@gmail.com
252. *Pestovskii Nikolai Valerievich*, LPI RAS, pestovsky@phystech.edu
253. *Petrik Galina Georgievna*, IGR DSC RAS, galina_petrik@mail.ru
254. *Petrov Yuri Vasilevich*, ITP RAS, uvp49@mail.ru
255. *Petrovskiy Victor Pavlovich*, JIHT RAS, b1p2a3@mail.ru
256. *Petukhov Vyacheslav Aleksandrovich*, JIHT RAS, +7(495)4858190, petukhov@ihed.ras.ru
257. *Pikuz Sergey*, JIHT RAS, +7(495)4841944, spikuz@gmail.com
258. *Pinchuk Mikhail Ernestovich*, IEE RAS, pinchme@mail.ru
259. *Pinevich Sergey Gennad'evich*, JIHT RAS, radical29@yandex.ru
260. *Pisarev Vasily Vyacheslavovich*, JIHT RAS, +7(495)4858545, pisarevvv@gmail.com
261. *Pogorelko Victor*, CSU, vik_ko83@mail.ru
262. *Pokrovskiy Georgy Vadimovich*, JIHT RAS, george.pokrovskiy@gmail.com
263. *Polyakov Dmitry Nikolaevich*, JIHT RAS, +7(495)4841810, cryolab@ihed.ras.ru
264. *Popel Sergey Igorevich*, IKI RAS, serg.i.popel@gmail.com
265. *Popov Vyacheslav Sergeevich*, JIHT RAS, SlavaPopov1991@yandex.ru
266. *Popova Tatyana Vasil'evna*, CSU, tatyana_maskaeva@mail.ru
267. *Povarnitsyn Mikhail Evgen'evich*, JIHT RAS, +7(495)4842456, povar@ihed.ras.ru
268. *Pridannikov Andrey*, Makeyev GRTs, bugs001@mail.ru
269. *Prokhorov Aleksandr Nickolaevich*, CIAM, +7(499)7636184, prokhorov@ciam.ru

270. *Prokhorov Alexander Evgeniyvich*, ICMM UB RAS, +7(342)2378312, alexproher@gmail.com
271. *Pugachev Leonid*, JIHT RAS, +7(495)4842456, puleon@mail.ru
272. *Pugacheva Daria*, JIHT RAS, sedyakina.d@gmail.com
273. *Pykhtina Anna Ivanovna*, JIHT RAS, pykhtina@yandex.ru
274. *Radchenko Andrey*, TSUAB, andrey-radchenko@live.ru
275. *Radchenko Pavel Andreevich*, TSUAB, radchenko@live.ru
276. *Rakhel Anatolii Dmitrievich*, JIHT RAS, +7(495)3625773, a_rakhel@mail.ru
277. *Rekhviashvili Sergo Shotovich*, IAMA, rsergo@mail.ru
278. *Rosmej Olga Nikolaevna*, GSI, +49(6159)711323, o.rosmej@gsi.de
279. *Rubtsov Ivan Andreevich*, LIH SB RAS, riv2112@mail.ru
280. *Rusin Sergey Petrovich*, JIHT RAS, +7(495)3625333, sprusin@yandex.ru
281. *Ryabinkin Alexey Nikolaevich*, SRC RF TRINITI, +7(495)9394953, alex.ryabinkin@gmail.com
282. *Ryazantsev Sergey Nickolaevich*, JIHT RAS, sergryaz@mail.ru
283. *Rychagov Aleksei*, FIPCE RAS, Rychagov69@mail.ru
284. *Rykov Sergey Vladimirovich*, SPbSU ITMO, togg1@yandex.ru
285. *Rykov Vladimir Alekseevich*, SPbSU ITMO, rykov-vladimir@rambler.ru
286. *Saakyan Sergey Aramovich*, JIHT RAS, saasear@gmail.com
287. *Safonova Daria Borisovna*, CIAM, safonova@ciam.ru
288. *Saitov Ilnur Minnigazievich*, JIHT RAS, saitovilnur@gmail.com
289. *Samoilova Anastasiia Alekseevna*, BMSTU, samoylova.nas@gmail.com
290. *Sargsyan Mikael Armenovich*, JIHT RAS, m.sargsyan86@mail.ru
291. *Sautenkov Vladimir Alexeevich*, JIHT RAS, vsautenkov@gmail.com
292. *Saveliev Andrey Sergeevich*, JIHT RAS, +7(495)4858063, fisteh@mail.ru
293. *Savintsev Alexey Petrovich*, KBSU, +7(8662)423777, pnr@kbsu.ru

294. *Savintsev Yurii Petrovich*, IGM SB RAS, +7(383)3332007, savincev1940@mail.ru
295. *Savitsky Dmitry Vladimirovich*, JIHT RAS, dmvlsav@yandex.ru
296. *Savoiskii Yurii Vladimirovich*, KBSC RAS, savoiskii@list.ru
297. *Scherbakov Konstantin Aleksandrovich*, MA SRT, rolikijin@mail.ru
298. *Schlothauer Thomas*, TUBAF, +49(3731)393540, schlotha@mineral.tu-freiberg.de
299. *Selyakov Ivan Nikolaevich*, JIHT RAS, ivan_sel@yahoo.com
300. *Semyonov Vladimir Pavlovich*, MIEM HSE, VPSemenov@gmail.com
301. *Serov Alexander Olegovich*, SRC RF TRINITI, +7(495)9394953, aserov@mics.msu.su
302. *Serpinsky Oleg Stanislavovich*, CIAM, surp9@mail.ru
303. *Sevrouk Kirill L'vovich*, HMTI NASB, +375(17)2841520, sevrouk@dnp.itmo.by
304. *Shakhray Denis Vladimirovich*, IPCP RAS, +7(496)5221756, shakhray@icp.ac.ru
305. *Shargatov Vladimir Anatolievich*, NRNU MEPhI, shargatov@mail.ru
306. *Shatan Ilya Nikolaevich*, HMTI NASB, +710(375)297161566, inshatan@gmail.com
307. *Shemakhin Aleksandr Yurievich*, KFU, shemakhin@gmail.com
308. *Shemanin Valery Gennad'evich*, KubSTU NPI, +7(8617)613291, vshemanin@mail.ru
309. *Shepelev Vadim Vladimirovich*, ICAD RAS, vadim.aries@gmail.com
310. *Shevchenko Arseny*, NRNU MEPhI, arsshevchenko@inbox.ru
311. *Shimchenko Sergey Yur'evich*, HMTI NASB, +375(29)5495546, sergey.shimchenko@gmail.com
312. *Shpakov Konstantin Victorovich*, LPI RAS, konstantine.shpakov@gmail.com
313. *Shpatakovskaya Galina Vasilievna*, KIAM RAS, +7(499)2507887, shpagalya@yandex.ru
314. *Shpekin Michael Ivanovich*, KFU, MichaelS1@yandex.ru
315. *Shumikhin Aleksey Sergeevich*, JIHT RAS, +7(495)3625310, shum_ac@mail.ru

316. *Shumova Valeria Valerievna*, JIHT RAS, +7(495)4842610, shumova@ihed.ras.ru
317. *Shutov Alexander Vladimirovich*, IPCP RAS, +7(496)5221447, shutov@ficp.ac.ru
318. *Sidorov Rodion Sergeevich*, CIAM, sidorov.rodion@gmail.com
319. *Sidorov Vladimir Sergeevich*, JIHT RAS, vladimir.sidorov.89@gmail.com
320. *Skobelev Igor Yurievich*, JIHT RAS, igor.skobelev@gmail.com
321. *Smirnov Evgeny Borisovich*, FSUE RFNC–VNIITF, ewgeny_smirnov@mail.ru
322. *Smirnov Vladimir Nikolaevich*, ICP RAS, +7(495)9397396, shumova@ihed.ras.ru
323. *Smygalina Anna Evgenievna*, JIHT RAS, anna.smygalina@gmail.com
324. *Sokotushchenko Vadim Nikolaevich*, JIHT RAS, sokotushenko@mail.ru
325. *Son Eduard Evgen'evich*, JIHT RAS, +7(495)4841655, utro-2007@mail.ru
326. *Sorokin Andrey Arturovich*, RDB named after A.Lyulka, Andrey.Sorokin@okb.umpo.ru
327. *Sosikov Vasiliy Aleksandrovich*, IPCP RAS, +7(49652)24125, vaso@icp.ac.ru
328. *Starikov Sergey*, JIHT RAS, redshuhart@yandex.ru
329. *Stegailov Vladimir Vladimirovich*, JIHT RAS, +7(495)4858545, stegailov@gmail.com
330. *Steinman Eduard Alexandrovitch*, ISSP RAS, +7(496)5228344, steinman@issp.ac.ru
331. *Stroev Nikita*, JIHT RAS, nikita.stroev@phystech.edu
332. *Struleva Evgenia Vyacheslavovna*, JIHT RAS, +7(495)2294240, struleva.evgenia@yandex.ru
333. *Stuchebrukhov Igor Alexandrovich*, GPI RAS, +7(499)5038300, st777@kapella.gpi.ru
334. *Sultanov Valery Gulyamovich*, IPCP RAS, sultan@ficp.ac.ru
335. *Sumskoi Sergey Ivanovich*, NRNU MEPhI, sumskoi@mail.ru
336. *Syrovatka Roman Aleksandrovich*, JIHT RAS, syrovatkara@gmail.com
337. *Sytchev George Alexandrovich*, JIHT RAS, +7(495)4857981, george.sytchev@gmail.com
338. *Talala Kseniya Anatolevna*, Makeyev GRTs, +7(3513)286102,

ktalala@yandex.ru
339. *Ten Konstantin Alekseevich*, LIH SB RAS, ten@hydro.nsc.ru
340. *Tereza Anatoly Mikhailovich*, ICP RAS, +7(495)9397396, atereza@bk.ru
341. *Ternovoi Vladimir Yakovlevich*, IPCP RAS, ternovoi@ficp.ac.ru
342. *Timofeev Alexey Vladimirovich*, JIHT RAS, +7(495)4859263, mail.timofeev.av@gmail.com
343. *Torchinskiy Vladimir Moiseyevich*, JIHT RAS, +7(495)4857981, torchvm@yandex.ru
344. *Torshhoeva Zeinap Sultanovna*, IngGU, torshhoeva.zina@yandex.ru
345. *Trigger Sergey Alexandrovich*, JIHT RAS, +7(495)3625310, satron@mail.ru
346. *Trubina Svetlana Vladimirovna*, IIC SB RAS, +7(383)3304447, svt@niic.nsc.ru
347. *Tsirlina Elena Arkad'evna*, JIHT RAS, Elena2509@yandex.ru
348. *Tsventoukh Mikhail Mikhailovich*, LPI RAS, +7(499)1322250, elley@list.ru
349. *Ushnurtsev Andrey Evgenevich*, IPCP RAS, ushnur@ficp.ac.ru
350. *Usmanov Ravil Anatolievich*, JIHT RAS, ravus46@yandex.ru
351. *Ustyuzhanin Evgueny Evguenyevich*, MAI, evgust@gmail.com
352. *Utkin Alexander Vasilievich*, IPCP RAS, +7(496)5224125, utkin@icp.ac.ru
353. *Uvarov Sergei Vitalievich*, ICMM UB RAS, +7(342)2378312, usv@icmm.ru
354. *Vagner Sergey Aleksandrovich*, IPCP RAS, vagnerserge@gmail.com
355. *Vasilyak Leonid Mikhailovich*, JIHT RAS, +7(495)4841810, cryolab@ihed.ras.ru
356. *Vaulina Olga Stanislavovna*, JIHT RAS, +7(495)4842355, olga.vaulina@bk.ru
357. *Vervikishko Daria*, JIHT RAS, vitkina-darya@yandex.ru
358. *Vervikishko Pavel Sergeevich*, JIHT RAS, pvervikishko@gmail.com
359. *Vetchinin Sergey Petrovich*, JIHT RAS, +7(495)4841810, uvlightsvp@yandex.ru
360. *Veysman Mikhail Efimovich*, JIHT RAS, bme@ihed.ras.ru

361. *Vikhrev Victor Victorovich*, RRC KI, INS, +7(499)1967703, vikhrev@mail.ru
362. *Vilshanskaya Evgeniya Vladimirovna*, JIHT RAS, eva.villi@gmail.com
363. *Vladimirov Vladimir Ivanovich*, JIHT RAS, +7(495)4842429, vld@ihed.ras.ru
364. *Vlasov Pavel Aleksandrovich*, ICP RAS, +7(495)9397396, iz@chph.ras.ru
365. *Volkov Nikolay Borisovich*, IEP UB RAS, +7(343)2678660, nbv@iep.uran.ru
366. *Vorob'ev Vladimir Sergeevich*, JIHT RAS, vrbv@mail.ru
367. *Vorob'eva Galina Yur'evna*, IPCP RAS, +7(49652)24473, vorobeva@icp.ac.ru
368. *Vorobiev Aleksey Aleksandrovich*, MA SRT, vorobievall@mail.ru
369. *Voronin Dmitriy Stanislavovich*, CSU, v-demonizerus@mail.ru
370. *Vshivkov Aleksei Nikolaevich*, ICMM UB RAS, aleksey.1992@mail.ru
371. *Yakovenko Ivan Sergeevich*, JIHT RAS, +7(495)4844433, yakovenko.ivan@bk.ru
372. *Yakovleva Ekaterina Alexandrovna*, UrFU, katrina.yakovleva@inbox.ru
373. *Yakushev Vladislav*, IPCP RAS, +7(49652)24125, yakushev@ficp.ac.ru
374. *Yankovsky Boris Denisovich*, JIHT RAS, yiy2004@mail.ru
375. *Yarantsev Dmitry Alekseevich*, JIHT RAS, yarantsev.d@gmail.com
376. *Yaroslavtsev Alexey*, UrFU, yaroslavtcev.a@mail.ru
377. *Yatsenko Pavel Ivanovich*, JIHT RAS, mr.pavl1kk@gmail.com
378. *Yaumenchikau Mikalai L'vovich*, HMTI NASB, +375(29)3554679, evmenchikov@mail.ru
379. *Yusupov Damir Ildusovich*, JIHT RAS, spt_yusupov@mail.ru
380. *Zaikin Sergey Vladimirovich*, CIAM, zaikin@ciam.ru
381. *Zaikova Vasilisa*, UrFU, vasilisazaykova@gmail.com
382. *Zakatilova Ekaterina Igorevna*, JIHT RAS, ei.zakatilova@mail.ru
383. *Zaponov Arseniy Eduardovic*, MA SRT, nopaz@mail.ru
384. *Zaporozhets Yury Borisovich*, IPCP RAS, +7(49652)21474, yubz@icp.ac.ru

385. *Zelener Boris Borisovich*, JIHT RAS, bobozel@mail.ru
386. *Zelener Boris Vigdorovich*, JIHT RAS, +7(495)4842333, zelener@ihed.ras.ru
387. *Zezyulina Tatiana*, FSUE RFNC–VNIIEF, +7(831)3028311, tat.zez@gmail.com
388. *Zhakhovsky Vasily Victorovich*, VNIIA(L), ceppera@gmail.com
389. *Zhilyaev Dmitry*, JIHT RAS, zhiliay@gmail.com
390. *Zhukov Andrey Nikolaevich*, IPCP RAS, +7(49652)21885, azhukov@icp.ac.ru
391. *Zhukov Pavel Andreevich*, VNIIA(S), trigun.forever@gmail.com
392. *Ziborov Vadim Serafimovich*, JIHT RAS, vziborov@rambler.ru
393. *Zobnin Andrey Vjacheslavovich*, JIHT RAS, zobnin@ihed.ras.ru
394. *Zolnikov Konstantin Petrovich*, ISPMS SB RAS, +7(382)2286972, kost@ispms.tsc.ru
395. *Zubareva Alla Nikolaevna*, IPCP RAS, +7(496)5224125, zan@ficp.ac.ru