BOOK OF ABSTRACTS

MOSCOW & CHERNOGOLOVKA & NALCHIK 2020

INTERNATIONAL CONFERENCE ON EQUATIONS OF STATE FOR MATTER

**MARCH 1–6 2020
ELBRUS
KABARDINO-BALKARIA
RUSSIA**

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The book consists of abstracts of plenary lectures, oral reports and posters presented at the XXXV International Conference on Equations of State for Matter (1–6 March 2020, Elbrus, Kabardino-Balkaria, Russia). The presentations deal with the contemporary investigations in the field of physics of extreme states of matter. The conference topics are as follows: equations of state and constitutive equations for matter under extreme conditions at high pressures and temperatures; shock waves, detonation and combustion physics; interaction of intense laser, x-ray and microwave radiation, powerful particle beams with matter; experimental techniques of generation and diagnostics of extreme states of matter; methods of mathematical modeling in physics of extreme states of matter; high-energy astrophysics; physics of low-temperature and non-ideal plasma; physical issues of power engineering and technology aspects.

The conference is supported by the Russian Academy of Sciences as well as the Kabardino-Balkar Scientific Center of the Russian Academy of Sciences.

The editorial board with deep regret announces the death of friends and colleagues: Professor Vladimir Ivanovich Molotkov (17 March 1941 – 11 July 2019); Corresponding Member of the Russian Academy of Sciences, Professor Sergey Ivanovich Anisimov (11 December 1934 – 15 October 2019); Doctor Vyacheslav Aleksandrovich Petukhov (6 February 1940 – 26 November 2019); Professor Alexander Borisovich Shvartsburg (26 January 1937 – 15 February 2020). All of them were active participants in the Conferences on Equations of State for Matter and Interaction of Intense Energy Fluxes with Matter.

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1. Equations of State
for Matter

$$\Gamma = (Z^2 e^2 / \varepsilon_{\mathrm{T}}) n_e^{1/3}$$

Fortov V E

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

fortov@ras.ru

Non-ideality parameter

$$\Gamma = \frac{Z^2 e^2}{\varepsilon_{\mathrm{T}}} n_{\mathrm{e}}^{1/3} \tag{1}$$

is discussed. Here Z is the average ion charge; e is the elementary charge; ε_{T} is the average kinetic energy of electrons; n_{e} is the electron number density.

Equation of state for yttrium at high pressures and temperatures

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 for yttrium is proposed with taking into account melting and evaporation effects. Calculations of thermodynamic characteristics and the phase boundaries of solid, liquid and gaseous Y over a wide range of densities and temperatures are carried out. Comparison of calculated results with available experimental data and theoretical predictions at high energy densities is presented. Obtained multiphase equation of state for yttrium can be used effectively in numerical modeling of processes under conditions of intense pulsed influences on the metal.

Lanthanum group: Detection and correction of errors in orbital binding energy measurements of internal shells

Shpatakovskaya G V

Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, Miusskaya Square 4, Moscow 125047, Russia

shpagalya@yandex.ru

Experimental data [1–3] on electronic binding energies in a ground state of lanthanides are analyzed. The data scatter is discussed. The method [4] using two universal functions $e(\sigma_n)$ and $d(\sigma_n)$ ($\sigma_n = \pi n Z^{-1/3}$, n is a main quantum number) is proposed to select more correct values.

Internal K, L, M, N individual shells are studied in detail. The dependence of the functions $e_n(\sigma_n)$ and $d_{nlj}(\sigma_n)$ on quantum numbers $n, l, j = l \mp 1/2$ (l is an angular quantum number) allows to analyze data taking into account relativistic effects.

The method makes it possible to show the law of similarity of binding energies by atomic number and to detect deviations from it in some experimental results, thereby indicating measurement errors.

Orbital binding energies as computed in the relativistic local-density approximation (RLDA) [5] for the lanthanides are also considered.

[1] Thompson A *et al* 2009 X-ray data booklet *Report* LBNL/PUB-490 Rev.3 (Berkeley, California 94720: Lawrence Berkeley National Laboratory)
[2] Naumkin A V, Kraut-Vass A, Gaarenstroom S W and Powell C J 2012 *NIST X-ray Photoelectron Spectroscopy Database. NIST Standard Reference Database 20, Version 4.1* URL http://dx.doi.org/10.18434/T4T88K
[3] Thomas D 1997 *Binding Energies of Electrons in Atoms* URL http://www.chembio.uoguelph.ca/educmat/atomdata/bindener/elecbind.htm
[4] Shpatakovskaya G V 2019 *Phys. Usp.* **62** 186–197
[5] Kotochigova S, Levine Z H, Shirley E L, Stiles M D and Clark C W 1997 *Phys. Rev.* A **55** 191

Phase transitions in the local equation-of-state approximation and anomalies of spatial ion profiles in non-uniform plasma

Chigvintsev A Yu[1,@]**, Iosilevskiy I L**[2,1]**, Noginova I Yu**[4] **and Zorina I G**[3]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[3] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia
[4] Russian State Agrarian University—Timiryazev Moscow Agricultural Academy, Timiryazevskaya 49, Moscow 127550, Russia

[@] alex012008@gmail.com

The impressive appearance of discontinuities in the equilibrium profiles of space charge in inhomogeneous Coulomb systems is discussed in a number of problems of thermoelectrostatics. Such discontinuities are considered as peculiar micro-level manifestation of phase transitions and intrinsic macro-level non-ideality effects in a local equation of state (EOS), which should be used for description of non-ideal ionic subsystem in frames of local-density (or "pseudo liquid", or "jellium" etc) approximation. Special emphasis is made in present paper on the mentioned above non-ideality effects in non-uniform ionic subsystems, such as micro-ions profile within screening cloud around macro-ion in complex (dusty, colloid etc) plasmas, equilibrium charge profile in ionic traps or (and) in the neighborhood vicinity of "charged wall" etc). Multiphase EOS for simplified ionic model of classical charged hard spheres on uniformly compressible electrostatic compensating background was constructed and several illustrative examples of discussed discontinuous ionic profiles were calculated.

Metastable states, metastable equilibria, and critical points in a simple one-component system

Baidakov V G[@] and Protsenko S P

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

[@] bai@itp.uran.ru

First-order phase transitions suggest the metastable state existence. Two phases, metastable with respect to a certain third phase, can coexist in equilibrium with each other on a flat interface. The latter means that in a single-component system, each of the three lines of phase equilibrium can be expanded beyond the triple point. Metastable extensions of the melting and sublimation lines meet, respectively, the spinodals of a stretched liquid and an overheated crystal. The contact points of these lines are singular: in the first case for the liquid and in the second for the crystalline phase. At the same time, they are not distinguished by anything for the phases coexisting with them.

In molecular dynamics experiments with Lennard-Jones systems, the thermodynamic parameters of the end points of the melting and sublimation lines have been determined. The stability conditions of the crystalline phase in the vicinity of the end point of the melting line have been considered. It is shown that a solid body reacts differently to spatially homogeneous and inhomogeneous deformations. At temperatures below that of the end point of the melting line, spinodal states are achievable. The phase decay of the crystalline phase here proceeds through the nucleation and growth of cavitation voids.

Homogeneous electron gas at finite temperatures and exchange-correlation functionals

Levashov P R[1,2,@] and Bonitz M[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 141701, Russia
[3] Institut für Theoretische Physik und Astrophysik, Leibnizstrasse 15, Kiel 24098, Germany

[@] pasha@jiht.ru

Electron gas has been attracting a lot of attention since the formulation of the Fermi statistics in 1926. The model of ideal (non-interacting) Fermi-gas has been formulated many years ago and is widely used in astrophysics, solid-state physics and some other fields. Account of Coulomb interaction, however, leads to very complicated theoretical problems unsolved up to now. For this reason numerical methods for electron gas are of particular importance. Traditionally the so-called jellium model of electron gas is considered in which quantum electrons are placed in the uniform non-compressible positive background. It is important to underline that well-known exchange-correlation energy in local approximation can be directly extracted from the equation of state of the jellium model. At $T = 0$ energy of the jellium model has been calculated using the diffusion Monte Carlo method [1]. However at finite temperatures one should apply quantum-statistical methods of simulation, such as path integral Monte Carlo. An overview of recent path integral simulations of the jellium model in wide range of temperatures and densities will be given and the problem of density function theory calculations at finite temperatures will be discussed.

[1] Ceperley D M and Alder B 1980 *Phys. Rev. Lett.* **45** 566

A multiphase equation of state for tin

Mikhaylov V N[@], Elkin V M and Mikhaylova T Yu

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

[@] v.n.mikhaylov@vniitf.ru

Two versions of the multiphase (the solid beta and gamma phases, liquid and vapor) equations of state for tin are constructed. They almost identically describe available experimental data on its thermophysical properties, and isothermal and shock compression, but give different melting curves at high pressures. Under shock compression, tin starts to melt at a pressure of 46.3 GPa (EOS46) in the first variant and at 59.7 GPa (EOS60) in the second one. The reason for our developing these two variants is the uncertainty that is present in the experimental data on tin melting on the shock wave.

Theoretical investigation of the shock compression of porous samples of metals

Kadatskiy M A[1,@] 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 141701, Russia

[@] makkad@yandex.ru

The results of calculations of the shock adiabats of porous samples of Al ($m_\mathrm{p} = 3$), Fe (1.825), Cu (4) and Mo (1.825) are presented. Here, $m_\mathrm{p} = \rho_0/\rho_{00}$, where ρ_0 is the normal density of the metal under consideration, ρ_{00} is the initial density of the porous samples. The calculations are carried out by the Thomas–Fermi with quantum and exchange corrections and the Hartree–Fock–Slater models with taking into account the ionic subsystem by the ideal Boltzmann gas and the charged hard spheres models in the pressure range from 10 to 10^7 GPa. The comparison of the calculation results with the available experimental data and with the calculation results of other models is given.

Measurement of the compressibility and temperature of shock compressed monocrystalline silicon up to 500 GPa

Nikolaev D N[@], Kulish M I, Dudin S V and Mintsev V B

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

Monocrystalline silicon is transparent in the near-infrared (ir) range
(1.2–8 μm). The affordable InGaAs photodiodes cover the range of
wavelengths 0.9–2.2 μm. It allows to register a thermal radiation
from shock wave front in silicon and various infrared-transparent
semiconductors in a manner, recently used to measure Hugoniot
temperatures of optically transparent materials like various crys-
tals and organic liquids. In this work, the samples of monocrys-
talline silicon were shock-compressed by means of traditional and
Mach-type explosive generators. Shock compressibility was deter-
mined by impedance matching with Quartz reference up to pressure
500 GPa. Brightness temperature of shock front was measured by 4-
channel near-ir pyrometer (1.3, 1.5, 1.6, 1.8 μm bands). The experi-
mental brightness temperature, measured in the pressure range 70–
500 GPa, demonstrates the strong disagreement (2–5 times lower)
between experimental data and equation-of-state predictions. Pos-
sible reasons of the observed difference will be discussed.

Calculation of shock-wave characteristics of multicomponent mixture by Hugoniot adiabates of polycrystalline components

Ostrik A V[@] and Nikolaev D N

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

A method of developing equations of state for a polycrystalline solids according to its experimental Hugoniot adiabat is proposed. The numerical method for determining specific cold energy and Grüneisen function at temperature $T = 0$ depending on the compression degree of the matter is considered.

The mix model for the multicomponent material and the numerical algorithm of its realization are described. When constructing equations describing dynamic behavior of the mix, two limit cases are considered [1]: ideal heat exchange which causes equalization of temperatures of mix components (isothermal approximation) and absence of heat exchange between its components (adiabatic approximation).

Unloading isentropes for shock compressed state of initially porous mixtures are given.

[1] Bakulin V and Ostrik A 2015 *Complex action of radiations and particles on the thin-walled constructions having heterogeneous coverings* (Moscow: FIZMATLIT)

On the effects of melting on the shock-wave compression of lead

Rakhel A D

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

rakhel@oivtran.ru

The Mie–Grüneisen equation of state is traditionally used to interpret the results of shock-wave experiments [1, 2]. In fact, in those works [1, 2] it is postulated that the equation of state has the Mie–Grüneisen form, and the dependence of the Grüneisen coefficient on the specific volume is taken from some model relation, whose accuracy is not exactly known. A different approach which does not use the model assumptions has been proposed recently [3]. In this paper, we use this approach and show that in the pressure range $P \leqslant 100$ GPa the equation of state of compressed lead indeed has the Mie–Grüneisen form. We determine for this pressure range directly from the experimental data on the shock compression of porous samples of lead the dependence of the Grüneisen coefficient on specific volume and check it for a singularity related to melting.

[1] Rice M H, McQueen R G and Walsh J M 1958 *Solid State Phys.* **6** 1
[2] Al'tshuler L V, Kormer S B, Bakanova A A and Trunin R F 1960 *Sov. Phys. JETP* **11** 573
[3] Rakhel A D 2018 *J. Phys.: Condens. Matter* **30** 295602

The sound velocity measurements for liquid lead in a wide range of density

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

A method was developed for measuring the sound speed in expanded liquid metals, including refractory ones, at high temperatures and pressures achieved in dynamic experiments [1]. In the experiments, the sample of the metal under study is a foil strip of 20–30 μm thickness, and 10 mm width and length, which is sandwiched between two plates of the window material (silica glass or sapphire). To measure the sound velocity an acoustic disturbance is excited (using a laser pulse) on the front surface of the foil strip at an instant t_1. The instant of arrival of this disturbance on the back surface of the foil t_2 is detected by a laser interferometer. The sound velocity is determined by the ratio $d(t_2)/(t_2 - t_1)$, where $d(t_2)$ is the sample thickness at the instant of arrival of the disturbance at the back surface of the sample. This measurement technique is developing by us during the past two years. Earlier we presented preliminary results of the sound velocity measurements in liquid iron [2] and liquid lead [3]. In this work, we demonstrate that for liquid lead this technique allows one to achieve a good reproducibility of the measurements results. The results obtained here on liquid lead were compared with literature data and errors of the present measurements have been estimated.

[1] Kondratyev A M, Korobenko V N and Rakhel A D 2018 *J. Exp. Theor. Phys.* **127** 1074–86
[2] Kaptilniy A G, Kondratyev A M, Pletnev A E and Rakhel A D 2018 *Vestnik Obedinennogo Instituta Vysokih Temperatur* **1** 36–9
[3] Kondratyev A M and Rakhel A D 2019 *XXXIV Int. Conf. on Interaction of Intense Energy Fluxes with Matter, March 1–6, 2019, Elbrus, Kabardino-Balkaria, Russia*

Estimation of three-dimensional effects in deformation of the window material plates in exploding foils experiments

Ivanov A V[@] and Rakhel A D

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

[@] avivanov_2@edu.hse.ru

Currently, methods for determining the pressure in dynamic experiments [1] are based on Hugoniot shock data [2]. However, in the experiments [1] the window material is compressed isentropically, so that at sufficiently high pressures this method of determining pressure may not be accurate enough. To determine the quantity accurately the Poisson adiabatic of the window material for the case of the uniaxial compression is needed. The experimental technique [1] allows one to determine this adiabatic with sufficient accuracy. As it turned out, errors of such measurements depend essentially on the correct evaluation of three-dimensional effects in the deformation of the window material.

In the work, equations of motion of a plane-parallel fused silica plate of finite thickness, width and length has been written and solved using the elasticity theory techniques. In this problem, a flat piston pushes one of the surfaces of the plate while the other surfaces are free.

[1] Kondratyev A M and Rakhel A D 2019 *Phys. Rev. Lett.* **122** 175702
[2] Barker L M and Hollenbach R E 1970 *J. Appl. Phys.* **41** 4208

Thermophysical properties of a lead–bismuth eutectic alloy in solid and liquid phases

Pletnev A E[@], Rakhel A D, Kondratyev A M and Kaptilnyi A G

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

[@] sanya.pletniov@yandex.ru

The Rosatom state corporation is developing the high-tech nuclear reactor SVBR-1000 with the lead–bismuth eutectic (LBE) as a coolant. However thermophysical properties of this alloy are known in very limited ranges of temperature and pressure, and often data obtained by different authors are not in agreement with each other [1]. In our laboratory we have developed a dynamic experimental technique which allows one to study thermophysical properties of conducting materials over sufficiently wide ranges of temperature and pressure [2]. To study the properties of a certain material in such dynamic experiment, a sample of the material is resistively heated by an electrical current pulse. However since the thermal expansion coefficient of the LBE in the solid state is negative, the integrity of the sample may be violated during the pulse heating, which will result in a non-uniform heating of the sample. In the present work, the resistivity of the LBE alloy in the solid and liquid state is measured using both the dynamic and a static experimental technique. In the latter the above feature of the LBE does not violate the sample integrity. Based on the present measurements results the errors of the measurements in the dynamic experiments have been estimated.

[1] *Handbook on Lead–Bismuth Eutectic Alloy and Lead Properties, Materials Compatibility, Thermalhydraulics and Technologies* (NEA)
[2] Kondratyev A M Korobenko V N and Rakhel A D 2018 *J. Exp. Theor. Phys.* **127** 1074

Modeling the thermodynamic properties of metal alloys at high energy densities

Seredkin N N[1,2,@] and Khishchenko K V[1,3]

[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] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] nikser12@yandex.ru

In this paper, we propose a model of the thermodynamic properties of alloys based on the equations of state of components. The main assumption is taken into account that in the states of thermodynamic equilibrium both mechanical and thermal equilibrium occur for all components of the alloy under consideration. The model is used to calculate the shock compressibility of metal alloys. The calculation results are compared with the available data of experiments with shock waves.

Possibilities for isentropic compression of metals by magnetic implosion of liners up to 30 Mbar

Buyko A M

Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia

ambuyko@vniief.ru

Review of experimental and computational papers is presented on generation of megabar isentropic compression of metal in the process of cylindrical liner implosion under action of azimutal magnetic field in the megagauss range [1–6]. The Al liner were investigated and, as a rule, two layer liners, the inner layer of which is the material studied (Fe, Cu, Ta, W), with the closely placed current carrying layer (Al, Cu), where the magnetic pressure is generated in the skin layer. High precision measurements of the inner surface velocity below 20 km/s for Al, Al–Cu, Al–Ta liners were presented in [1]. New computational technique based on experiments was also developed to reconstruct isentrops of metals up $\sim$ 10 Mbar with several percents accuracy. The analogous technique was developed and approbated for implosion Al, Al–W and Cu–W liners in magnetic explosive systems [4,6]. The explosive systems with Al, Al–W and Cu–W liners imploded by magnetic fields up to 118 MG (magnetic pressure up to 13 Mbar) isentropic compression of metals to pressure $\approx$ 30 Mbar were investigated in [2, 3, 5]. Results obtained in these papers with some new ones are discussed.

[1] Lemke R W, Dolan D H *et al* 2016 *J. Appl. Phys.* **119** 015904
[2] Buyko A M 2017 *Proc. Int. Conf. XX Khariton Scientific Talks* 143–52
[3] Bazanov A A, Baranov V K and Buyko A M *et al* 2019 *Proc. Int. Conf. XX Khariton Scientific Talks* 143–52
[4] Garanin S F, Kuznetsov S D *et al* 2018 *16th Megagauss Conf.*
[5] Buyko A M, Ivanova G G and Morozova I V 2019 *Proc. Int. Conf. XXI Khariton Scientific Talks* 234–8
[6] Karepov V A and Kuznetsov S D 2020 *This book of abstracts*

Computational equation of state parameters reconstruction in experiments with disk explosive magnetic generators to study properties of metals under shockless compression up to 10 Mbar

Kuznetsov S D[@] and Karepov V A

Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia

[@] SDKuznetsov@vniief.ru

Some possibilities were investigated to study shockless compression of materials to megabar pressure with the disk explosive generator systems (DEMG) with a foil opening switch (FOS) [1, 2]. It is possible to obtain isentropic compression of materials to pressure more than 10 Mbar [3]. Estimate of the equation of state (EOS) parameters is presented in this paper for different samples from Cu, W, Ta shocklessly compressed with pushers from Al and Cu to high pressures. Modeling was made of experiments to study material properties with different EOS parameterizations for the synthesized experimental inner liner surface velocities. The accuracy of reconstructed EOS parameters was obtained based on the expected precision of velocity measurements with the photon Doppler velocimetry. The procedure used is based on running one-dimentsional computations in the shell of optimizers like BOX and DAKOTA, which make possible EOS parameters optimization.

[1] Kuznetsov S D, Garanin S F *et al* 2018 *16th Int. Conf. on Megagauss Magnetic Field Generation and Related Topics*
[2] Karepov V A and Kuznetsov S D 2019 *11th Int. Conf. on Dense Z-Pinches (DZP 2019)*
[3] Buyko A 2020 *This book of abstracts*

Thermodynamic functions of dense plasmas with pseudoatom molecular dynamics

Ovechkin A A[@], Falkov A L and Loboda P A

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

[@] ovechkin.an@mail.ru

Thermodynamic functions of aluminum have been calculated along several isochores using pseudoatom molecular dynamics—classical molecular dynamics with pair interatomic potentials obtained in the framework of the Starrett and Saumon average-atom model allowing for ion correlations [1]. Calculated isochores are compared to the simulation data obtained with quantum molecular dynamics and path integral Monte Carlo methods [2]. Ionic contributions to the thermodynamic functions are compared to the results of one-component-plasma simulations.

[1] Starrett C E and Saumon D 2016 *Phys. Rev. E* **93** 063206
[2] Driver K P, Soubiran F and Militzer B 2018 *Phys. Rev. E* **97** 063207

Thermodynamic properties of C–N–O–H mixture in the region of non-ideal plasma

Rykounov A A[@] and Vorobyova M A

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

[@] arykounov@gmail.com

The atmosphere of giant planets in the Solar System, such as Uranus and Neptune, consists of mixed water, ammonia, and methane heated to the state of warm dense matter. All these compounds have rather complicated phase diagrams which include some exotic structures, e.g., super-ionic water. A physically consistent description of all interactions in such mixtures can only be attained from first principles. The non-empirical methods, such as quantum molecular dynamics (QMD), are however strongly limited both in the dimensions of systems which can be modeled, and in the times during which their evolution can be tracked. We try to tackle these problems by modifying the classical reaction potential ReaxFF [1] on the basis of the pair correlations functions obtained in QMD calculations. Here we investigate how the calculated thermodynamic properties of mixed carbon, nitrogen, oxygen and hydrogen depend on ReaxFF parameters for systems of several tens of thousand atoms, and do comparisons with similar results obtained from first principles for much smaller systems.

[1] Strachan A and van Duin A C T 2003 *Phys. Rev. Lett.* **91** 098301

Crystal potentials and thermophysical characteristics of solidified inert gases

Kyarov A Kh[@] and Savintsev A P

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

[@] pnr@kbsu.ru

The construction of reliable state equations in a wide range of temperatures, pressures and the consideration of surface phenomena for various condensed matter, is currently an urgent problem. When determining the thermophysical characteristics of solidified inert gases using Lennard-Jones potentials, significant discrepancies with experiment were revealed, which problems when studying the properties of a substance under extreme conditions.

An interpolation model is proposed for paired modified potentials, including dipole–dipole and dipole–quadrupole contributions, and the thermophysical characteristics of molecular crystals are studied. The possibility of determining the parameters of a model crystalline potential in the additive approximation of pair interaction by numerical methods has been shown [1]. The "cold" equations, surface energy, and surface tension of crystals of solidified inert gases are investigated. In the high-temperature approximation, the dependences of the volume and coefficient of isothermal compressibility on temperature and pressure, and the dependence of the critical temperature on pressure for solidified inert gases were calculated [2, 3]. The results obtained are in good agreement with experimental data.

[1] Kyarov A Kh, Temrokov A I and Khaev B V 1997 *High Temp.* **35** 380–4
[2] Bourne M and Kun H 1954 *Dynamical Theory of Crystal Lattices* (Clarendon Press)
[3] Melikyan A O, Pogosyan L A and Saakyan S M 1992 *Phys. Solid State* **34** 611–7

Semiclassical calculation of porous copper shock Hugoniots

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

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya 22, Moscow 127055, Russia

[@] serj.dyachkov@gmail.com

Being well-studied, copper is widely used in shock-wave physics as a reference material in high velocity impact experiments. Nowadays, impact velocities may exceed 20 km/s [1] resulting in shock pressures of several TPa; such extreme conditions allow us to validate simplified theoretical models. A variety of approaches to construct such models exist from the most simple ideal Boltzmann gas for ions and Fermi gas for electrons to computationally expensive self-consistent density functional theories. In the middle, an average atom framework combined with the charged hard spheres ion model may provide adequate description of electron subsystem in copper [2]. Instead of the Hartree–Fock–Slater (HFS) model used for electrons in shock Hugoniot calculations [2], a less computationally expensive approach with semiclassical wave functions is used to account shell effects caused by the bound electrons [3]. Our results are compared to the experimental data on shock compression of solid and porous copper samples and HFS calculations.

[1] McCoy C A, Knudson M D and Root S 2017 *Phys. Rev. B* **96** 174109
[2] Kadatskiy M A and Khishchenko K V 2018 *Phys. Plasmas* **25** 112701
[3] Dyachkov S A, Levashov P R and Minakov D V 2016 *Phys. Plasmas* **23** 112705

Thermodynamic coefficients of ideal Fermi-gas

Kozharin A S[1,2,@] and Levashov P R[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 141701, Russia

[@] 1alekseik1@gmail.com

Equation of state (EOS) of ideal Fermi-gas (IFG) [1] describes thermodynamic properties of a system of non-interacting electrons and is widely used in astrophysics and condensed matter theory. Also IFG model is important for practical computations with a chemical picture approach and as a constituent of a wide-range EOS. The functional form of IFG EOS usually consists of the non-linear dependencies of free energy and particle density on temperature; both equations contain chemical potential as a parameter. Therefore for practical applications different approximations of IFG free energy are used providing correct asymptotes at zero and high temperatures. The uncertainty of thermodynamic functions calculated using such approximations may be significant, especially for the so-called thermodynamic coefficients or second derivatives of free energy. In this work we propose a python module `ifg-py` [2] that calculates thermodynamic functions of IFG using high-accuracy approximations of Fermi-integrals [3]. The module can be applied in a wide range of temperatures and particle densities and returns first and second derivatives of free energy as well as a number of thermodynamic functions including heat capacity and sound velocity.

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Semiclassical estimation of ionization degree in the Thomas–Fermi model for a mixture of elements

Krasnova P A[1,@] **and Levashov P R**[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 141701, Russia

[@] pakrasnova@gmail.com

In the traditional way of estimating the average ionic charge in the models of the middle atom, it is assumed that the dependence of the electron density on the radius of the spherical cell is constant. Therefore the mean ion charge in this case can be calculated as the product of electron density on the boundary of the cell and the volume of the cell. Although the effects of temperature and pressure ionization as well as full ionization are reproduced this procedure is quite rough and can substantially overestimate the ionization degree especially for heavy elements. In this work we implemented a semiclassical method of mean ion charge estimation [1] in which the Thomas–Fermi dependence of electron density on the radius of a spherical cell is taken into account. The method is applied to the Thomas–Fermi model for a mixture of elements [2]; special attention is paid to the region of low densities where conventional chemical picture models are valid. An improved evaluation of ionization degree may be crucial for simulation of absorption of laser radiation by plasma.

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Surface energy of low-melting alloys and graphite intercalated with potassium in the framework of the Thomas–Fermi model using the results of molecular-dynamic modeling

Akhmatov Z A[1,@] **and Khokonov A Kh**[1,2]

[1] Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia
[2] Kabardino-Balkar Scientific Center of the Russian Academy of Sciences, Inessa Armand 37, Nalchik, Kabardino-Balkaria 360051, Russia

[@] ahmatov.z@bk.ru

The surface energy of low-melting alloys, as well as graphite intercalated by potassium atoms, was calculated using the Thomas–Fermi–Dirac electronic-statistical model [1, 2]. The initial ion distribution was found using molecular dynamics simulation using the LAMMPS program. For metals and their alloys, surface energy calculations were carried out both for oriented crystalline planes and for spherical clusters. The calculations of the surface energy of the liquid metal–intercalated graphite interface indicate a decrease of surface energy with an increase of potassium concentration in graphite interlayer space.

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Thermodynamics of refractory metals in the near-critical region by ab initio calculations

Minakov D V[1,2,@], Paramonov M A[2,1] and Levashov P R[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 141701, Russia

[@] minakovd@ihed.ras.ru

We present comprehensive first-principle study of thermodynamic properties of liquid tungsten (W) and molybdenum (Mo) in the near-critical region. The first *ab initio* estimates of the critical parameters of W and Mo based on quantum molecular dynamics calculations of supercritical isotherms are also provided. The robustness of our calculations is confirmed by excellent agreement with available experiments on isentropic expansion of shock-compressed porous samples and several experiments on isobaric expansion of pulse-heated wires. We also present isochoric and isobaric heat capacity, the Grüneisen coefficient, the critical isobar and the speed of sound in the liquid refractory metals up to the critical point. A significant growth of isochoric and isobaric heat capacities of liquid W and Mo along the critical isobar while approaching the critical point is observed in our calculations. On the other hand, the Grüneisen parameter noticeably decreases along the critical isobar and reaches the value at the critical point that is much lower than the ideal gas limit of $\gamma = 2/3$. This result is consistent with some previous experimental works for aluminum [1] and lead [2].

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Thermodynamic properties of liquid uranium: Ab initio simulation and interpretation of experimental data

Paramonov M A[1,2,@]**, Minakov D V**[1,2] **and Levashov P R**[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 141701, Russia

[@] mikhail.a.paramonov@phystech.edu

Equation of state of uranium is of great importance for analyzing the nuclear safety of existing nuclear reactors or planned for operation in the future, including modeling hypothetical conditions that can lead to severe man-made accidents and their consequences. However, the near-critical region of the uranium phase diagram is not available for precise experimental study because of high temperatures and high pressures. Theoretical description of this region is hampered by the complicated electronic structure of uranium and strong Coulomb interaction. Thus, it seems that at present the only available theoretical approach that can provide thermophysical information for a warm expanded liquid metal is the first-principle method of quantum molecular dynamics (QMD) based on the electron density functional theory.

The purpose of this work is to study some thermodynamic properties of uranium in the vicinity of the boundary of the two-phase liquid–gas region using the QMD method. In this work an original interpretation of experimental data on isobaric expansion, shock compression of porous samples and subsequent isentropic expansion of uranium is presented. The influence of relativistic effects on the thermodynamic properties is also analyzed.

Method of evaluation of the soft-spheres potential parameters for calculating entropy in molecular dynamics simulations

Barsukova A 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 141701, Russia

[@] anastasiya.barsukova@phystech.edu

There are two main approaches for calculating entropy in atomistic modeling. This is the Widom test particle method [1] and the thermodynamic integration method [2]. Both methods are accurate, but technically difficult and require a large number of calculations. Therefore, in 2003, a new method for the approximate calculation of entropy based on the results of only one molecular-dynamic simulation was proposed [3]. The authors proposed the so-called two-phase model, in which the studied system was divided into two subsystems: solid and gas. To describe the gas phase, the model of hard spheres was used. But further analysis shows that the two-phase model is not accurate enough in calculating entropy for refractory metals. Therefore, in this work we propose the model of soft spheres for describing the gas part. The approach [4] will be used to determine the parameters of the repulsive part of the potential from the *ab initio* structure factor of molybdenum. Further steps will be discussed to describe the gas part of the system under study and to calculate the entropy using the two-phase model.

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Equation of state of boron carbide at high pressures and temperatures from quantum molecular dynamics simulations

Rykounov A A

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

arykounov@gmail.com

Boron carbides are promising materials for creating high-strength body armor due to their relatively low density and very high micro-hardness. Due to high chemical and mechanical resistance they are widely used in other industry and technology branches (as refractory material, abrasives, etc).

In the report, we used quantum molecular dynamics (QMD) method to calculate the local equation of state for the stoichiometric boron carbide B_4C. The statical properties up to pressures 20 Mbar are examined and shown that the phase transition on the $T = 0$ isotherm resulting in amorphization occurs at pressure about 143 GPa. For both the solid and porous materials Hugoniots were obtained and compared with existing experimental data.

Ultrastiffness of diamond on the nanoscale: A first-principles study

Khabibrakhmanov A I[1,2,3,@] **and Sorokin P B**[1,2,3]

[1] National University of Science and Technology "MISIS", Leninskiy Avenue 4, Moscow 119049, Russia
[2] Technological Institute of Superhard and New Carbon Materials, Tsentralnaya Street 7a, Troitsk, Moscow 108840, Russia
[3] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] almaz.khabibrakhmanov@phystech.edu

Diamond crystal is well-known for its unique mechanical properties having the highest bulk modulus and being referred to as the hardest crystalline material. Search for materials beating diamond by their mechanical properties draws close attention of materials scientists and attempts to find such materials continue through decades to this day [1]. Nanodiamonds (or diamond nanoclusters) represent several nm in size diamond particles. The size effects in such clusters lead to a modification of the original diamond properties. Structural, electronic and magnetic properties of nanodiamonds attract significant interest and have been studying for many years [2]. Some recent experimental evidence also exists [3], showing that nanodiamonds are superior to diamond by mechanical stiffness. For the first time, we carried out an extensive first-principles study of nanodiamonds structural and mechanical properties in a wide range of shapes and sizes (35–1798 atoms). We obtained that there is an increase in both bulk modulus B_0 and average bonds stiffness k_0 for studied structures comparing to bulk diamond values. Also, we investigated the advantages and limitations of the average bonds stiffness approach. Finally, we explained the nature of nanodiamonds stiffening and showed that k_0 is a convenient and unambiguous physical quantity describing mechanical properties of covalently bonded nanostructures.

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Ab initio study of MgO under pressure using quasiharmonic approximation

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

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] burov.as@phystech.edu

In this work, we examine the behavior of the Gibbs free energy and entropy on pressure and density along MgO isotherm 300 K. Earlier, some theoretical works [1, 2] predicted a drastic drop of entropy by analyzing existing experimental data and extrapolating them to high pressures. We have performed first-principle calculations of thermodynamic properties of MgO under pressure using density functional theory and quasiharmonic approximation. The robustness of our calculations has been verified by comparing the calculated and experimental phonon dispersion curves. The comparison with available diamond anvil cell experimental data is also provided. Our estimate for the B1–B2 phase transition is in good agreement with other experimental and theoretical studies [3]. However, our results for the entropy do not agree with previous calculations [1,2] in which an expression containing the coefficient of thermal expansion and isothermal bulk modulus is integrated by volume at $T = 300$ K. Possible causes of discrepancies are analyzed and discussed.

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Equations of state of CaSiO$_3$ polymorphs for the Earth's upper mantle conditions

Sokolova T S[@] and Dorogokupets P I

Institute of the Earth's Crust of the Siberian Branch of the Russian Academy of Sciences, Lermontov Street 128, Irkutsk 664033, Russia

[@] sokolovats@crust.irk.ru

We have constructed equations of state for 3 polymorphic modifications of CaSiO$_3$: wollastonite ($V_0 = 39.9$ cm^3/mol), pseudowollastonite ($V_0 = 40.2$ cm^3/mol) and walstromite ($V_0 = 37.8$ cm^3/mol). The proposed equations of state are based on the Helmholtz free energy where thermal part of the free energy is presented by the Einstein model with two characteristic temperatures by analogy with our previous studies [1,2]. The Einstein characteristic temperatures are estimated from measurements of heat capacity at low and intermediate temperatures and entropy at standard temperature. The reference isotherm is determined by the Kunc equation [3]. The fitting parameters of the equations of state are determined by the least squares method in the Excel spreadsheets. The derived equations of state are allowed to calculate of all thermodynamic functions (heat capacity, entropy, bulk modules, Gibbs energy, etc) for minerals depending on temperature and volume or temperature and pressure. The equilibrium lines (wollastonite–pseudowollastonite and wollastonite–walstromite) are calculated and can be used to study of structure and composition of the Earth's upper mantle.

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Sapphire anvil cell for Raman high-pressure studies at elevated temperatures

Sayfulin M Zh[1,2,@], Sholin I A[1] and Orlov N S[1]

[1] Institute of Solid State Physics of the Russian Academy of Sciences, Akademika Osipyana Street 2, Chernogolovka, Moscow Region 142432, Russia
[2] Lomonosov Moscow State University, Leninskiye Gory 1, Moscow 119991, Russia

[@] sayfulinmarsel@yandex.ru

The basic method of studying the behavior of various substances in our laboratory at pressures up to 9 GPa is by using the so-called thermobaric quenching. First, the sample is equilibrated at the pre-selected pressure and temperature in a large-volume high-pressure chamber made of a superhard WC alloy. After the equilibrium is reached, which takes from a few minutes to a few days depending on the experiment, the sample is rapidly cooled (quenched) to the liquid nitrogen temperature together with the high-pressure chamber. In many cases, cooling to the N_2 temperature freezes the phase composition of the synthesized sample that allows its further investigation in a metastable state at ambient pressure and cryogenic temperatures using Raman spectroscopy, x-ray and neutron diffraction, etc. The main objective of our current efforts is to supplement these ex situ investigations with in situ studies by Raman spectroscopy in the same pressure range up to 9 GPa and elevated temperatures using large-volume sapphire anvil cells. To date, we have achieved 5.5 GPa and 70 °C.

Chemical reactions in the iron–water system at high pressures

Prokoshin A V[1,2,@] and Efimchenko V S[1]

[1] Institute of Solid State Physics of the Russian Academy of Sciences,
Akademika Osipyana Street 2, Chernogolovka, Moscow Region 142432, Russia
[2] Lomonosov Moscow State University, Leninskiye Gory 1, Moscow 119991,
Russia

[@] prokoshin.artem@gmail.com

Our studies of a fayalite–hydrogen system at pressures up to 7.5 GPa and a ratio of H_2 to Fe_2SiO_4 equal to 2.2 revealed the formation of water, iron and a small amount of hematite (Fe_2O_3). It was assumed that the formation of hematite due to the reaction of water with iron that were formed after the fayalite decomposition in the high-pressure cell. To verify this assumption, the iron powder was pressurized at $t = 280$ °C with distillated and deionized water up to $P = 7.5$ GPa and exposed at these conditions for 24 h. Further the pressure and temperature were released to the ambient conditions and the sample was studied by x-ray diffraction, Raman spectroscopy and energy dispersive x-ray spectroscopy (EDX). The x-ray diffraction pattern was contained only the bcc iron diffraction peaks. However, our Raman spectroscopy and EDX studies showed the formation of Fe_2O_3 compound on the surface of iron particles.

Solid solutions of molecular hydrogen in amorphous calcium silicates

Pogosyan P Z[1,2,@] **and Efimchenko V S**[1]

[1] Institute of Solid State Physics of the Russian Academy of Sciences, Akademika Osipyana Street 2, Chernogolovka, Moscow Region 142432, Russia
[2] Lomonosov Moscow State University, Leninskiye Gory 1, Moscow 119991, Russia

[@] pogosyanpz@gmail.com

Powders of the amorphous calcium silicates Ca_ySiO_{2+y} at $y = 0.15$, 0.225, 0.3, 0.67 were produced by a sol-gel method followed by sintering at 700 °C. The bulk samples of $Ca_{0.225}SiO_{2.225}$ and $Ca_{0.67}SiO_{2.67}$ glasses were synthesized by the quenching of corresponding melts. According to results of the energy dispersive x-ray spectroscopy (EDX), the space distribution of calcium cations in the initial silicate samples with $y = 0.15$, 0.225 and 0.3 were substantially heterogeneous. However, in according to x-ray diffraction data, all samples were amorphous and no contain any crystalline impurities. The samples were hydrogenated at $P = 7.5$ GPa and $t = 250$ °C, quenched to the liquid N_2 temperature to prevent hydrogen losses after the pressure release and further studied in the quenched state at ambient conditions by x-ray diffraction and Raman spectroscopy. The molar ratio of H_2 of the samples was determined by hot extraction into a pre-evacuated volume.

Reactions in the fayalite–deuterium system at high pressures

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

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

[@] efimchen@issp.ac.ru

Hydrogen-induced decomposition of fayalite (Fe_2SiO_4) at high pressure is of considerable interest for understanding the chemical processes occurring in the Earth's mantle and inside icy satellites. To study the effect of the amount of hydrogen present in the system, the fayalite (Fa) samples were deuterated at $P = 7.5$ GPa and $t = 280$ °C with the preset molar ratios of D_2 to Fa (D_2/Fa) equal to 1, 1.5, 2.2 and 5 in the reaction cell. The deuterated samples were further quenched to the liquid N_2 temperature to prevent hydrogen losses after the pressure release and further studied in the quenched state at ambient conditions by x-ray diffraction, Raman spectroscopy and quadrupole mass-spectroscopy. Experiment showed that the high-pressure deuteration led to the chemical decomposition of fayalite via breaking the Fe–O bonds and was always accompanied by the formation of heavy water. The solid products of the reaction varied from a mixture of ferrosilite ($FeSiO_3$) and iron at D_2/Fa = 1 to a mixture of silica and iron at D_2/Fa = 2.2.

Anisotropic thermal deformation and first-order phase transition in crystals 2,4,6-trinitrotoluene and 2,4-dinitroanisole

Rudina A Kh[1], Stankevich A V[1,@], Kostitsyn O V[1], Garmashev A Yu[1], Taibinov N P[1], Filyakova V I[2], Rusinov G L[2], Rasputin N A[2] and Kvashnin Yu A[2]

[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] Postovsky Institute of Organic Synthesis of the Ural Branch of the Russian Academy of Sciences, Sofia Kovalevskaya Street 22, Ekaterinburg 620137, Russia

[@] alexvstankevich@mail.ru

This paper presents the studies of thermal deformation tensors and the first-order phase transition for two energetic materials: α-2,4,6-trinitrotoluene (α-TNT) and α-2,4-dinitroanisole (α-DNAN), calculated according to x-ray powder diffraction within the temperature range from 150 to 355 K for α-TNT and from 150 to 370 K for α-DNAN. We obtained ultrapure α-TNT samples by sublimation purification of the initial TNT, and α-DNAN samples by alcoholysis of 2,4-dinitrochlorobenzene with the subsequent recrystallization and sublimation purification. We recorded structural changes of energetic materials by thermal x-ray diffraction methods of the internal standard with a step of 10 and 2 K (near the melting point). We studied the long-range and short-range order of the crystalline state of the objects under study in the field of the first-order phase transition. We calculated powder x-ray diffraction data by full-profile methods with the integrated into algorithm cycle of quantum simulation of molecules and crystals structure. As a result, we defined the main crystallographic axes and characteristic surfaces of thermal deformation tensor presented numerically, algebraically and graphically.

Analysis of anisotropic thermal expansion for 2,4,6-triamino-1,3,5-trinitrobenzene crystals by single and powder x-ray diffraction

Stankevich A V[1],[@], Slepukhin P A[2], Rusinov G L[2], Kostitsyn O V[1] and Taibinov N P[1]

[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] Postovsky Institute of Organic Synthesis of the Ural Branch of the Russian Academy of Sciences, Sofia Kovalevskaya Street 22, Ekaterinburg 620137, Russia

[@] alexvstankevich@mail.ru

The paper presents x-ray diffraction experiments for determining of the state of TATB (2,4,6-triamino-1,3,5-trinitrobenzene) crystal at finite temperatures. We studied monocrystal samples at three temperature points 100, 200 and 298 K. Data on monocrystal diffractometry at certain were processed by SHELXL algorithms. Powder samples were studied over the range from 150 to 550 K with a step of 10 K. Data on powder thermal x-ray radiography of the internal standard were handled with the help of full-profile methods with the quantum-topology structural model of molecules and crystals integrated into accounting cycle. We aligned experimental points of 200 and 298 K with the subsequent calibration of the curve of quasi-isobaric expansion of TATB powder. As a result, we obtained thermal deformation tensors of TATB crystals and more accurate estimates of coefficient of its anisotropic thermal expansion.

Thermal deformation of detonation diamonds within the range of 150–550 K

Taibinov N P, Stankevich A V[@], Kostitsyn O V and Garmashev A Yu

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

[@] AlexVStankevich@mail.ru

The paper presents precision analysis of thermal expansion of ultra-dispersed diamonds obtained by detonation synthesis under different conditions. We determined coefficients of thermal expansion (compression) on the basis of powder thermal x-ray radiography of the internal standard with a step of 20 K, built the tensors of thermal deformation of ultradispersed diamond crystal structure. Besides, we revealed the dependence of thermal deformation on the initial state of the samples: defect structure, nitrogen doping degree and presence of polytrophic carbon shell. We calculated experimental data by full-profile analysis methods with integrated cycle of quantum simulation of crystal structure. As the result we determined the main crystallographic axes and characteristic surfaces of thermal deformation tensor presented numerically, algebraically and graphically. The obtained results can be used while developing physical and mathematical description of the condensed ultradisperse diamonds behavior under thermal impact.

Investigation of the electronic structure of metals and carbon materials by annihilation spectroscopy methods in low-background Baksan Neutrino Observatory conditions

Taer M S[1,@]**, Khokonov A Kh**[1,2,3]**, Gangapshev A M**[1,2] **and Akhmatov Z A**[1]

[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
[3] Kabardino-Balkar Scientific Center of the Russian Academy of Sciences, Inessa Armand 37, Nalchik, Kabardino-Balkaria 360051, Russia

[@] mavar2014@yandex.ru

Currently, positron annihilation spectroscopy methods are finding wider application for solving the problems of restoring the electronic structure of matter [1]. Earlier, in NIKA laboratory of the Baksan Neutrino Observatory, we conducted an experiment to measure the gamma activity of the $\omega = 1454$ keV line of the ^{40}K isotope after intercalation of pyrolytic graphite with potassium atoms [2]. We used the Doppler spectroscopy of annihilation peak to determine the radius of the Fermi surface of metals and carbon materials, including graphite intercalated by potassium atoms. Spectra of annihilation photons were obtained for samples of metals Ag, Cu, W, Au, Pb, as well as for polyethylene, pure and intercalated with potassium atoms, pyrolytic graphite. This work was supported by the grants of Russian Foundation for Basic Research No. 18-02-01042 and the Fund for the Promotion of Innovation No. 0038507.

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The use of electromagnetic forces to control the capillary properties of eutectic gallium alloys droplets

Sergeev I N[1,@], Khokonov A Kh[1,2,3] and Akhmatov Z A[1]

[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
[3] Kabardino-Balkar Scientific Center of the Russian Academy of Sciences, Inessa Armand 37, Nalchik, Kabardino-Balkaria 360051, Russia

[@] pirlfix@mail.ru

Eutectic alloys of gallium with indium and tin are able to maintain a fluid state at room temperatures and, unlike mercury, have low toxicity. For the technological use of gallium alloys, methods are being developed for electrochemical [1] and electromagnetic effects [2] on their capillary properties. In this paper, we present the results of a study of the microliter drops of Ga–In and Ga–Sn eutectic alloys capillary properties on a conductive substrate in a uniform magnetic field when a direct current is passed through the substrate. It was found that for the investigated alloys, the contact angle in the magnetic field changes significantly, while the magnitude of the effect is proportional to the current and magnetic field induction. The influence of ponderomotive forces is reduced to the additional pressure normal to the surface of the droplet and pressing it to the substrate. When the contact angle is above 90° the applying of constant magnetic field lead to increase of contact angle with the rise of electrical current along the droplet surface. In the case when the initial contact angle corresponds to good wetting the ponderomotive forces also pressed the droplet to substrate whereas the contact angle decreases that can be used for improving the soldering. This work is supported by grant No. 18-02-01042 from the Russian Foundation for Basic Research.

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Fe–V–Al alloys under high pressure: Thermoelectric and electrical properties

Korobeynikov I V[1,@], Usik A Yu[1], Marchenkov V V[1,2] and Govorkova T E[1]

[1] Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, Sofya Kovalevskaya Street 18, Ekaterinburg 620219, Russia

[2] Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

[@] i_korobeynikov@mail.ru

In this work, we discuss results of experimental investigation of Seebeck coefficient (S) and electrical conductivity behavior under high pressure (P) up to 10 GPa for Fe–V–Al alloys with L2$_1$-structure: near-stoichiometric compounds $Fe_{2-x}V_{1+x}Al$ and aluminum-poor $Fe_{2.43}V_{1.27}Al_{0.3}$.

High pressure investigation were carried out at room temperature using an automated set-up operating miniature anvil-type high-pressure cell with anvils made of hard-alloys [1].

We find that even small variations of composition can significantly change conduction type, $S(P)$ behavior and even reversibility of high-pressure effects.

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The effect of changing ratio of the transition elements on electroresistivity and magnetoresistivity of Fe–V–Al alloys

Usik A Yu$^{1,@}$, Okulov V I^1, Govorkova T E^1, Lonchakov A T^1, Emelyanova S M^1 and Marchenkov V V^{1,2}

^{1} Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, Sofya Kovalevskaya Street 18, Ekaterinburg 620219, Russia
^{2} Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

$^@$ alexandr-usik1990@rambler.ru

To clarify the role of the change in the ratio of transition elements in $Fe_{1.76}V_{1.2}Al_{1.04}$ and $Fe_{1.87}V_{1.1}Al_{1.03}$ alloys, studies of electrical and magnetoresistance were carried out at temperatures from 2 to 300 K and in magnetic fields up to 90 kOe. Alloys had the same Al content, but different in the composition in Fe and V, the ratio of which varied from 1.47 in the $Fe_{1.76}V_{1.2}Al_{1.04}$ to 1.7 in the $Fe_{1.87}V_{1.1}Al_{1.03}$ alloy. We found that when the temperature changes from 2 to 300 K, the electrical resistance of the $Fe_{1.76}V_{1.2}Al_{1.04}$ sample decreases by 1.7 times, and its magnetoresistance in the entire temperature range, and does not exceed 1%. Although the $Fe_{1.87}V_{1.1}Al_{1.03}$ alloy has an electrical resistance drop of 19 times, its magnetoresistance is negative and reaches 11% at low temperatures.

The observed differences in the behavior of the kinetic properties of the studied alloys can be related to the features of the electronic energy spectrum in the form of a narrow pseudogap at the Fermi level, the appearance of defects [1], which is a consequence of a change in the Fe-to-V ratio in the $Fe_{1.76}V_{1.2}Al_{1.04}$ and the $Fe_{1.87}V_{1.1}Al_{1.03}$ alloys from 1.47 to 1.7 respectively. This work was carried out as part of the state task of the Minobrnauki of Russia (theme "Electron" No. AAAA-A18-118020190098-5), and with partial support from the Russian Foundation for Basic Research (project No. 18-32-00618).

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Features of amorphization and crystallization of metal alloys under high pressure torsion

Sundeev R V[1,@], Shalimova A V[2], Glezer A M[2] and Rassadina T V[1]

[1] MIREA—Russian Technological University, Vernadskogo Avenue 78, Moscow 119454, Russia

[2] Bardin Central Research Institute for Ferrous Metallurgy, Radio Street 23/9 Bldg 2, Moscow 105005, Russia

[@] sundeev55@yandex.ru

Among the many unusual phenomena accompanying severe plastic deformation, the processes of amorphization deformation and crystallization deformation are of particular importance. The amorphization behavior of the crystalline multicomponent alloys based on Ti, Ni, Zr and Fe upon high pressure torsion (HPT) has been studied. It is shown that the crystalline to amorphous transition is determined by the ability of the crystals to accumulation of deformation defects under mechanical action, by the thermodynamic stability of the crystalline phases contained in the alloy, and by the possibility of the diffusion processes necessary for the change in the chemical composition of the crystalline and amorphous phases upon deformation. Specific features of the crystallization of amorphous alloys based on Fe during HPT have been studied at room temperature. It is found that the volume fraction of the crystalline phase formed in each of the amorphous alloys during deformation increases when its crystallization temperature decreases. The obtained results are explained on the assumption of adiabatic heating in shear band and also the hypothesis regarding an increase in the concentration of excess free volume regions in shear bands during deformation. This work was supported by the Russian Foundation for Basic Research (project No. 20-32-70007).

Universal structural and dynamic features in metals near their melting points

Khusnutdinoff R M

Kazan Federal University, Kremlyovskaya Street 18, Kazan, Tatarstan 420008, Russia

khrm@mail.ru

This paper presents the results of a comparative analysis of experimental data on the structural and dynamic properties and characteristics of liquid alkaline (Li, Na, K), alkaline earth (Mg, Ca, Sr) and transition metal groups—elements of the subgroups of nickel (Ni Pd, Pt) and copper (Cu, Ag, Au)—near their melting points. Reduced spatial $r/r_m = rk_m/(2\pi)$ and time $t/t_m = tk_m/\sqrt{m\beta}$ scales, in which k_m is the position of the main maximum of the static structure factor $S(k)$ and $\beta = 1/(k_B T)$ (k_B is the Boltzmann constant) is the inverse temperature, are introduced as the basis for the law of corresponding states. Based on these scale transformations and experimental data on x-ray diffraction, it was found that the groups of liquid alkaline, alkaline earth, and transition metals are described by universal r and k-dependencies. It has been established that the dispersion law of longitudinal polarization $\omega_c(k)$, given in accordance with these scale relations, for elements of groups of liquid alkaline, alkaline earth and transition metals has a single universal character. An analysis of the properties of three groups (alkaline, alkaline earth and transition) liquid metals using scale transformations shows that the law of the corresponding states is valid for these substances.

Physical and crystallographic basis of reversibility in shape memory alloys

Adiguzel O

Firat University, Elazig 23169, Turkey

oadiguzel@hotmail.com

Several alloy systems exhibit a peculiar property called the shape memory effect. This property is characterized by the recoverability of two certain shapes of material at different temperatures. The physical and crystallographic basis of this phenomenon is two successive crystallographic transformations; thermal induced and stress induced martensitic transformations; and these transformations are characterized by changes in the crystal structure of the material. Shape memory effect is result of successive thermally and stress induced martensitic transformations. Thermal induced martensitic transformation occurs on cooling along with lattice twinning by means of lattice invariant shears in two opposite directions, $\langle 110 \rangle$-type directions on the {110}-type plane of austenite matrix, and ordered parent phase structures turn into twinned martensite structures. By applying external stress, the twinned structures turn into detwinned martensite structures by means of strain induced martensitic transformation. Copper based alloys exhibit this property in metastable-phase region, which has bcc-based structures at high temperature parent phase field. Lattice invariant shear and twinning is not uniform in copper based ternary alloys and gives rise to the formation of complex layered structures, depending on the stacking sequences on the close-packed planes of the ordered parent phase lattice. In the present contribution, x-ray diffraction and transmission electron microscopy (TEM) studies were carried out on two copper based CuAlMn and CuZnAl alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections inherited from parent phases.

Experimental study of thermal expansion of chromium near its melting point

Senchenko V N[@] and Belikov R S

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

[@] pyrolab@ihed.ras.ru

Millisecond electric pulsed heating is a well-known method for studying refractory metals at high temperatures. Meanwhile, some properties of such materials, especially chromium, are still insufficiently investigated at this temperature region.

This work contains the experimental study of the temperature dependences of thermophysical properties of chromium at high temperatures and in the melting region by pulse electrical heating. Using this method, an experimental determination of the thermal expansion coefficient, electrical resistivity and emission spectra at premelting region of chromium have been carried out.

The obtained temperature dependences of the thermophysical properties of chromium are of interest, in particular, for constructing wide-range equations of state, as well as for use in high-temperature engineering.

Electrical resistivity of zirconium carbide at 1200–2500 K

Kostanovskiy A V[@], Kostanovskaya M E, Zeodinov M G and Pronkin A A

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

[@] kostanovskiy@gmail.com

Zirconium carbide produced from nanosized powders is a new material; its properties have not, in fact, been studied. We present the experimental results on the electrical resistivity of the zirconium carbide within the temperature range of 1200–2500 K. The ZrC specimens were prepared by spark plasma sintering from nanosize particles at a temperature of 2100 K. The goal of the present work is to compare the obtained results with data for ZrC produced by traditional methods.

Hafnium carbide evaporation in the vicinity of the melting point

Bardina T L[@], Frolov A M, Falyakhov T M and Petukhov S V

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

[@] bardina_1994@mail.ru

Hafnium carbide is an ultra high temperature ceramic (UHTC) with a very high melting point—4255 K [1]. Like other carbides of the metals of group IV hafnium carbide exhibits a combination of useful properties: high melting temperature, hardness, electric and thermal conductivity. Such features of HfC make it a promising material to be used under extreme conditions, for example in aerospace technology. For such applications one need to know experimental values on thermophysical properties at very high temperatures. However the study of evaporation behavior of the substance was carried out by stationary methods only for the solid state [2]. In the paper the results on the investigation of evaporation of liquid HfC are presented for the first time. The analysis of evaporation was conducted using time-of-flight mass-spectrometry combined with the heating with laser pulses of a millisecond duration. It was found that the evaporation of HfC occurs mainly through the dissociation of the carbide into hafnium and carbon atoms. Moreover small quantities of C_2, Zr and HfC are present in the vapor. Temperature dependences of relative partial pressures of different vapor species were obtained. The evaporation enthalpies and the temperature dependences of the ratio of carbon and hafnium atoms were calculated. It was found that the C-to-Hf atomic ratio tend to a value of 0.22 at temperatures above 4300 K.

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On using the ratio temperature to estimate the true temperature of an emitting material

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 method (gray model) is presented for estimating the true temperature of an opaque emitting material, both above and below, with an unknown character of the spectral emissivity dependence. It is shown that if in the selected spectral range the graph of the spectral distribution of inverse radiance temperatures can be approximately represented by a line convex down then the obtained value of the ratio temperature limits the true temperature from above. If in the spectral interval the graph of the indicated dependence can be represented by a line convex up then the obtained value of the ratio temperature limits the true temperature from below. The solution to this inverse problem must be combined with the solution to the direct problem. As a result, additional information appears on the spectral distribution of the material emissivity in the selected spectral range. Besides, this is a verification of the assumptions made. An example of processing experimental data known from literary sources is given.

To the question of equations of state for heterogeneous media

Mishin A V[1,2]

[1] Khristianovich 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

alekseymishin1994@gmail.com

The present work is devoted to the study of the influence of heterogeneity on transport coefficients, which is reflected in the equation of state of matter. The main research methods [1,2] are the variational method, the self-consistent field method, and statistical models in the theory of effective modules. Based on these approaches, the effect of heterogeneity on the transfer coefficients is monitored, taking into account the presented characteristics of the phases (physical, geometric and topological). In the framework of these approaches the concept of the effective dimension of a heterogeneous system is introduced, which takes into account the mechanism of formation of effective degrees of freedom in it. As an example, the viscous properties of a heterogeneous liquid–solid phase system are studied, where the latter is a spherical inclusion. With increasing concentration of the solid phase the latter begins to be locally more and more connected and the viscosity of the system begins to increase more intensively. This happens in such a way as if the number of degrees of freedom in the system is less than 6 (the dimension of the system is less than 3), that is, the field selectively propagates over the phases of the medium. This circumstance is associated with the geometry of the analyzed system—balls, stochastically filling the space and having viscosity coefficients significantly exceeding the viscosity coefficients of the liquid phase. Based on this introduction, better agreement with the experiment is obtained than when considering a system with dimension 3.

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Large-scale molecular dynamics simulation of plastic deformation

Pokatashkin P A[@] and Yanilkin A V

Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya 22, Moscow 127055, Russia

[@] p.a.pokatashkin@gmail.com

Molybdenum is an important material for both practical and theoretical purposes. Very high melting of Mo (2896 K) on the one hand make it a promising structural material, on the other hand a wide pressure and temperature range of the bcc phase stability provides wide simulational opportunities. It is, therefore, a good example for development and calibration of elastic-plastic models.

We perform large scale molecular dynamics simulations of uniaxial compression of Mo along $\langle 100 \rangle$ direction. Strain rates 10^7–10^9 s^{-1} are considered. Contribution of various hardening mechanism are studied with respect to various strain rates and temperatures to produce a continuum dislocation dynamics (CDD) model. We emphasize that this approach does not require experimental data. The CDD results are in good agreement with various shock-waves experiments.

Structure and electronic properties of semimetallic crystalline molecular hydrogen at high pressures

Norman G E[1,2] **and Saitov I M**[2,1,@]

[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, Myasnitskaya 20, Moscow 101000, Russia

[@] saitovilnur@gmail.com

Semimetallic states of crystalline molecular hydrogen are obtained at a temperature of 100 K in a pressure range from 410 to 626 GPa. To analyze the nature of the conductivity, the band structure is calculated within the framework of the density functional theory using the HSE hybrid exchange-correlation functional. One of the semimetallic states arises in a monoclinic structure with C2/c symmetry upon compression to a pressure of 410 GPa, at which the gap between the valence band and the conduction band is closed. Moreover, the valence band is partially unfilled, and the conduction band is partially filled, which is a characteristic sign of *semimetal*. At a pressure of 302 GPa, crystalline molecular hydrogen with a C2/c structure remains an insulator. The pressure dependence of electrical conductivity is found for 300–500 GPa. The second semimetallic state is observed for a orthorhombic structure with Cmca-4 symmetry at a pressure of 626 GPa. The work is supported by the Russian Science Foundation (grant No. 18-19-00734).

Superconducting critical temperature of a novel phase of crystalline hydrogen

Obzhirov A E[1,2,@] **and Saitov I M**[1,2,3]

[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 141701, Russia
[3] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

[@] obzhirov.ae@phystech.edu

The superconducting critical temperature T_c is the temperature at the point at which the metal phase and the superconducting phase are in equilibrium. The value of T_c is solely determined by a crystal structure and can be predicted by first-principles methods. One way to calculate T_c is to use the semi-empirical McMillan formula [1], which is derived assuming certain shape of a phonon density of states. We study whether the McMillan formula can be used for the CMCA phase of metallic molecular hydrogen predicted to be stable at high pressures [2]. We calculate the phonon density of states of the new phase and compare it with the McMillan assumptions. We conclude that the McMillan formula is not applicable in our case and discuss the possibility of calculating T_c through the Eliashberg equations [3].

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Phase diagram and conductivity of warm dense argon

Sartan R 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 141701, Russia

r.sartan@gmail.com

The warm dense argon is studied by the *ab initio* molecular dynamics method in the framework of the theory of the density functional. The equations of state and conductivity of both the liquid and solid phases are calculated in the temperature and pressure ranges of 2000–25 000 K and 1–3500 GPa. No phase transition in the liquid phase is detected.

A maximum of the melting line is found near 15 GPa and 12 000 K. Conductivity increases smoothly with increasing temperature at densities up to 10 g/cm^3 and does not changes at higher densities. This behavior is consistent with [1]. Solid argon is also conductive at high temperatures.

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The molecular dynamics study of grain boundary migration in pure Ni

Korneva M A[1,@], Zhilyaev P A[1], Akhatov I S[1], Zhilyaev A P[2] and Starikov S V[3,4]

[1] Skolkovo Institute of Science and Technology, Skolkovo Innovation Center Bldg 3, Moscow 143026, Russia
[2] Ruhr-University Bochum, Universitaetsstrasse 150, Bochum 44801, Germany
[3] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[4] Institute for Metals Superplasticity Problems of the Russian Academy of Sciences, Stepana Khalturina Street 39, Ufa, Bashkortostan 450001, Russia

[@] marijakorneva@yandex.ru

In the present work, molecular dynamics (MD) simulations of pure Ni crystallites were performed to show the influence of the grain boundary (GB) geometry on the values of the activation energy of GB migration E_a [1,2]. The simulated systems were: bicrystal with 5[010] tilt plane boundary, spherical precipitate with initial curvature radius 5 nm, and polycrystalline $30 \times 30 \times 30$ nm^3 block. The motion of three types of GBs (flat, spherical, and polycrystalline) at constant temperatures and no applied forces was studied and compared. The derived values of E_a are 0.45, 0.11 and 0.57 eV, which is in consistence with theoretical explanations of triple-junction and curvature effects. Nevertheless, these values are smaller than derived in experimental works, which is common problem for all MD simulations of GB migration [3].

The special part of this work was the development of a script for the automated analysis of the polycrystalline structure. The derived code provided accurate analysis of each particular grain evolution.

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Precise calculations of hydrocarbons viscosities using classical molecular dynamics methods

Kondratyuk N D[1,2,@] **and Pisarev V V**[1,2]

[1] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] nkondratyuk@hse.ru

The shear viscosity coefficient is one of the key subjects of molecular modeling studies since this quality is used in the development of lubricants. In this work, we apply the molecular dynamics methods for predicting the liquid hydrocarbons viscosities at pressures up to 1 GPa [1–4]. The different classical force fields are compared by their predictive power. The COMPASS class II force field is chosen for the precise calculations. Both equilibrium and non-equilibrium methods are used to calculate the shear viscosities. The super-Arrhenius behavior of the pressure viscosity dependence is observed for 1,1-diphenylethane.

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Surface energy and viscosity of atomic nuclei at finite temperatures

Khokonov A Kh[1,2,3]

[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
[3] Kabardino-Balkar Scientific Center of the Russian Academy of Sciences, Inessa Armand 37, Nalchik, Kabardino-Balkaria 360051, Russia

azkh@mail.ru

Earlier [1], the viscosity of nuclear matter was estimated by comparing the experimental nuclei frequencies for octupole and quadrupole vibrations with the hydrodynamical model. In this work, we calculated the surface energy and the viscosity for even-even spherical nuclei on the base of finite Fermi systems model [2].

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A new code for computations of the thermodynamic functions of diatomic ideal gases

Maltsev M A[1,2,@], Morozov I V[1,2] and Osina E L[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 141701, Russia

[@] maksim.malcev@phystech.edu

Databases on the thermodynamic properties of materials play a significant role in solving engineering problems associated with the design of rocket engines, the creation of new materials, the development of chemical technologies, metallurgy, mining, waste processing, etc. Significant contribution to the solution of these problems was made by the information system IVTANTHERMO [1]. According to the basic principles formulated for IVTANTHERMO system, information in thermodynamic databases should be regularly updated. The development of new methods for calculating thermodynamic functions and programs that implement them are necessary to solve this problem. The calculation of the thermodynamic functions of diatomic molecules is traditionally based on the use of molecular constants. However, this method can be improved by using the interatomic interaction potential that is obtained by quantum chemical methods. This work presents a new code for calculating the thermodynamic properties of diatomic ideal gases based on this approach. All stages of calculation of basic thermodynamic functions in the temperature range 298.15–10 000 K are shown by examples of argon diatomic compounds [2–4].

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Equation of state for homogeneous systems

Osmanova B K[@], Bazaev E A and Bazaev A R

Institute for Geothermal Research and Renewable Energy—Branch of the Joint Institute for High Temperatures of the Russian Academy of Sciences, Shamilya 39a, Makhachkala, Dagestan 367030, Russia

[@] badji@mail.ru

From our experimental data on the p–T–ρ (pressure–temperature–density) relationship for homogeneous binary and ternary systems consisting of water, aliphatic alcohol (methanol, ethanol, and n-propanol) and hydrocarbons (n-pentane, n-hexane, n-heptane, n-octane) in sub- and supercritical states [1,2] compressibility factors and single-phase (liquid, vapor) critical and supercritical regions of state parameters are determined. From experimental data on the p–T–ρ relationship of the systems are described by a three-parameter polynomial equation of states, i.e., the expansion of compressibility factor $Z = P/(RT\rho)$ (where R is the gas constant) into series in powers of reduced density; reduced temperature and composition x (as the mole fraction of alcohol). The coefficients were determined via a generalized least squares method [3]. The average percentage errors of the calculated pressure values relative to the experimental values are 2% (liquid phase), 0.7% (vapor phase), and 0.5% (supercritical fluid).

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Equation for determination of decomposition points of pure alcohols and their aqueous mixtures

Dzhapparov T A G[@], Bazaev A R and Osmanova B K

Institute for Geothermal Research and Renewable Energy—Branch of the Joint Institute for High Temperatures of the Russian Academy of Sciences, Shamilya 39a, Makhachkala, Dagestan 367030, Russia

[@] timur507@mail.ru

Usage of homogeneous binary mixtures that consist of components with different boiling temperatures and critical parameters as heat-carriers or solvents in heat-and-power engineering and extraction setups is a perspective direction of widering of working parameters (temperature, pressure) range. Advantage of binary mixtures in comparing with pure components is that one can change their critical parameters by choosing the substances and their composition for realizing the technology processes in the wide diapason of temperatures and pressures. And for accurate calculating the parameters of heat-and-power engineering and extraction setups that use unstable components (for example, aliphatic alcohols) one must know the region of their thermal stability, especially the values of decomposition points. In this work, we experimentally determined experimental values of decomposition points (T_d) of pure alcohols (methanol, ethanol, 1-propanol and 1-butanol) and their aqueous mixtures (0.2, 0.5, 0.8 mole fractions of alcohol). The dependence of T_d of alcohol molecules in their aqueous mixtures from their concentration (x) and the carbon number (C) can be estimated by next polynomial equation.

Inflection point of the potential curve, potentials "companion": Critical parameters forecast

Petrik G G

Institute for Geothermal Research and Renewable Energy—Branch of the Joint Institute for High Temperatures of the Russian Academy of Sciences, Shamilya 39a, Makhachkala, Dagestan 367030, Russia

galina_petrik@mail.ru

The results obtained for the equation of state based upon the model of interacting point centers justified a new stage of research at the molecular level. Introduction to the description of the inflection point of the potential curve (PC) allowed obtaining a general relation, which related four parameters—coordinates of special points—minimum and inflection of PC—and indices n, m, determining the shape of potentials of the Mie family (m–n). Several variants of reading the general coupling equation have been proposed. It was interesting to use them in the analysis of potentials recovered from the second virial coefficient and viscosity. Analysis of the results for 10 molecules globules—n indices for the potential of Mie (n–6) and the coordinate values of the minimum potential—revealed some problems, which were the source of data for WF_6. Their decision required the introduction of the concept of two PC-"companions" characterizing each object. For one of them (with a large value of n) the critical temperature is better predicted, for the other (with a smaller value of n)—the critical volume. The obtained results clarify the association of the PC inflection point coordinates with the critical parameters set by us earlier. The general equation of communication allows explaining the anti-bath dependence of parameters of model potentials recovered by properties of substances noted by many authors.

Method of modeling the line of phase equilibrium of individual substances

Kudryavtseva I V[1,@], Rykov S V[1], Sverdlov A V[1], Ustyuzhanin E E[2] and Rykov V A[1]

[1] ITMO University, Kronvergskiy 49, Saint-Petersburg 197101, Russia
[2] National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

[@] neva0175@mail.ru

The question of modeling the line of phase equilibrium of individual substances for which experimental information is not available in a wide neighborhood of the triple point is discussed. The method is based upon the modified Clapeyron–Clausius equation $\rho^-(T) = p'_s(T)T/r^*(T)$ and an equation

$$p'_s(T)/p_s(T) = r^*(T)/(RT^2), \tag{1}$$

which follows from Clapeyron–Clausius equation under the condition that the substance on the vapor branch of the saturation line behaves in the vicinity of the triple point like an ideal gas. Here ρ^- is the density on the saturation line at $\rho < \rho_c$; ρ_c is the critical density; $p_s = p_s(T)$ is the saturated steam pressure; $r^* = r/(1-\rho^-/\rho^+)$; r is the heat of vaporization; ρ^+ is the density on the saturation line at $\rho > \rho_c$.

At the first stage, the parameters of modified Clapeyron–Clausius equation are calculated, then the functions $r^*(T)$ and $p'_s(T)$ are substituted into equation (1) and the equation $p_s = p_s(T)$. The calculations are repeated until the values of $p_s(T)$, $p'_s(T)$, $r^*(T)$ are agreed in a wide neighborhood of the triple estrus. To determine ρ^+ we use the rule of rectilinear diameter $(\rho^+ + \rho^-)/2 = A\tau + \rho_c^*$, $\tau = 1 - T/T_c$ which is valid outside the vicinity of the critical point (ρ_c, T_c, p_c). We calculate the density ρ_c^* taking into account the rule $(\rho^+ + \rho^-)/2\rho_c - 1 = a\tau^{2\beta} + b\tau^{1-\alpha} + \ldots$, where α and β are the critical parameters. The method was tested on the example of calculation in the phase equilibrium line R134a, R218 and R1234yf.

Method for calculating the equilibrium properties of pure substances based on the Migdal phenomenological theory

Rykov S V[1], Sverdlov A V[1], Ustyuzhanin E E[2], Rykov V A[1,@] and Nurysheva M[1]

[1] ITMO University, Kronvergskiy 49, Saint-Petersburg 197101, Russia
[2] National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

[@] rykov-vladimir@rambler.ru

In mathematical modeling of the thermodynamic surface, the pseudocritical point method based on the Migdal phenomenological theory and the Benedek hypothesis was widely used [1]. In this paper, we have significantly expanded the working range of equations of state [2] based on the pseudocritical point method [1]. The approach is based on the expression for the chemical potential μ

$$(\rho_c/p_c)[\mu(\rho, T) - \mu_0(T)]K_T^{\frac{\gamma+\beta}{\gamma}} = \sum_{n=1}^{3} \varphi_{2n-1}m^{2n-1} \tag{1}$$

and expression of the Helmholtz free energy F:

$$F(\rho, T) = F_{\text{reg}}(\rho, T) + f(\rho, T)|\Delta\rho|^{\delta+1}a_0(x) \tag{2}$$

where, ρ_c, p_c are critical parameters; $\mu_0(T)$, $f(\rho, T)$ and $F_{\text{reg}}(\rho, T)$ are regular functions; $\Delta\rho = \rho/\rho_c - 1$; $K_T = A|\Delta\rho|^{-\gamma/\beta}|x + x_1|^{-\gamma}$ [2]; $m = \Delta\rho K_T^{\gamma/\beta}$; α, β, γ and δ critical indices; x is the scale variable. The scale function $a_0(x)$ is calculated based on the expression (1) [1]. We tested the fundamental equation of state (2) using the example of modeling the thermodynamic surface of a number of substances: R32, R23, R1234yf, SF$_6$. The results are discussed.

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Joint processing of data on the coexisting densities and the meniscus position between two phases in the critical region of SF$_6$

Ustyuzhanin E E[1,@]**, Ochkov V F**[1]**, Popov P V**[4]**,**
Rykov V A[2]**, Rykov S V**[2] **and Lecoutre C**[3]

[1] National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia
[2] ITMO University, Kronvergskiy 49, Saint-Petersburg 197101, Russia
[3] Centre National de la Recherche Scientifique, Rue Michel Ange 3, Paris 75016, France
[4] All-Russian Research Institute of Metrological Service, Ozernaya Street 46, Moscow 119361, Russia

[@] evgust@gmail.com

This report considers some problems, which are connected with the behavior of the meniscus. The last separates the liquid and gas phases of a sample for a substance. This sample is placed in a sealed cell and heated up at a constant volume. The cell is a horizontal cylinder, which has a diameter, $d = 10.606$ mm. The position of the meniscus is determined as its height, h, over the volumetric median plane of the cell. The experiment [1] gave an (h, T) array related to SF$_6$. It is shown that the function, $y(\tau) = h/r$, can take values in the range, $y = -0.04$ to 0.03, if the temperature, $\tau = (T - T_c)/T_c$, decreases in the interval, $\tau = 10^{-2}$ to 10^{-6}. We have considered a number of problems: to investigate $y(\tau)$ theoretically at $\tau = 10^{-2}$ to 10^{-6} and at the microgravity ($g_m < g = 9.8$ m/s^2) as well as to evaluate (ρ_l, ρ_g, τ) data of SF$_6$ accordingly to experimental (y, τ) data [1]. It is built $y(\tau) = f(\mathrm{ur}, d)$, here $\mathrm{ur} = f_d/f_s$ is the complex, f_s is the order parameter, f_d is the mean diameter of the coexistence curve. These new (ρ_l, ρ_g, τ) data made it possible to form a modified array of (ρ_l, ρ_g, T) data as well as to build some models of (f_d, f_s) on the bases of this array.

[1] Garrabos Y, Lecoutre C, Marre S, Beysens D and Hahn I 2018 *Phys. Rev. E* **97** 020101

Fundamental equation of the state of SF$_6$, taking into account the next approximation of scale theory

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

ITMO University, Kronvergskiy 49, Saint-Petersburg 197101, Russia

[@] togg1@yandex.ru

Based on an expression for entropy S

$$\Delta S = X^{-\frac{1-\alpha}{\chi}} \left(\varphi_0 + \varphi_1 m^2 + \varphi_2 X^{-\frac{\Delta}{\chi}} + \varphi_3 X^{-\frac{\Delta}{\chi}} m^2 \right), \qquad (1)$$

and hypotheses about the nature of the behavior of thermodynamic functions that have a feature at a critical point

$$X = A|\Delta\rho|^{-\frac{\chi}{\beta}}|x + x_1|^{-\chi} \qquad (2)$$

a fundamental equation of state (FEoS) for sulfur hexafluoride has been developed.

Here $\Delta S = (\rho_c T_c/p_c)[S(\rho, T) - S_r(\rho, T)]\phi(\rho)$; ρ_c, p_c, T_c are critical parameters; $S_r(\rho, T)$ is the regular temperature T and density ρ function; $\phi(\rho)$ is the crossover function; α, β and Δ are critical indices; χ is the index that coincides with the critical index of the thermodynamic function X (for example, if $X = C_V$, then $\chi = \alpha$); $m = \Delta\rho X^{\beta/\chi}$; x is the scale variable; φ_n are constant coefficients.

In contrast to the FEoS [1], the following approximation of the scale theory of the critical point is taken into account in expression (1). Tables are calculated for pressure, isochoric and isobaric heat capacity, sound velocity, isothermal compressibility coefficient. A comparison is made with known thermodynamic tables of SF$_6$.

[1] Kudryavtseva I V, Rykov V A and Rykov S V 2019 *J. Phys.: Conf. Ser.* **1385** 012009

Investigation of the filtration process of methane–n-pentane mixture

Molchanov D A

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

dmitriy.molchanov13@gmail.com

The results of physical simulation of a one-dimensional isothermal process of filtration of a model binary gas-condensate mixture, which consisted of methane and n-pentane, are presented. The conditions under which non-stady filtration modes arise are determined. It is shown that retrograde properties of the model mixture leads to the appearance of self-oscillatory modes of gas-condensate fluid filtration.

Diffusion of ions in water solution of ethylene oxide polymers

Bakulin I K[1,2,@]**, Kondratyuk N D**[3,2]**, Lankin A V**[1,2] **and Norman G E**[1,2,3]

[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 141701, Russia
[3] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

[@] bakulin.ik@phystech.edu

We study the ionic conductivity of linear ethylene oxide polymers in aqueous solution using classical molecular dynamics methods. The simulated polymer chain has the length of 100 ethylene oxide units (C_2H_4O). Different interaction potentials are considered to reproduce the real behavior of solution. Polymer–water and polymer–ion interactions are validated. The diffusion coefficients of system components are derived using Einstein–Smoluchowski relation. We investigate the relation between diffusivity of ions and mass fraction of polymer in water solution and concentration of ions in the system. The work was prepared within the framework of the HSE University Basic Research Program and funded by the Russian Academic Excellence Project '5-100' (N D Kondratyuk) and grant No. 18-19-00734 of the Russian Science Foundation (I K Bakulin, A V Lankin, G E Norman).

Modeling the ternary system water–urea–sugar for storage systems of extremely large capacity

Deshchenia V I[2], Lankin A V[1,2,@] and Norman G E[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 141701, Russia

[@] alex198508@yandex.ru

The operation of power plants with solar and wind energy is highly dependent on meteorological conditions. The problem can be solved by incorporating electricity storage systems into the network. Requires the use of storage systems of extremely large capacity. One of the options for such systems can be flowing redox elements. In this regard, it is of interest to study transport processes in systems including carbohydrates, simple and complex, water and the third component, which is either a metal salt or other organic substance. Compounds that are sugars chemically bonded to organic structures capable of participating in redox reactions can be very interesting. One of the possible methods allowing us to approach the solution of this range of issues is the molecular dynamics method. It has already found wide application for the description of organic compounds, including sugars and polymer structures based on them. However, this approach always requires a thorough preliminary verification of the selected force field for the possibility of a fairly accurate description of the system parameters of interest. Using the molecular dynamics method, the properties of a water–urea–sugar ternary solution are considered in this work. The dependence of its thermodynamic parameters on the ratio of components is studied and a comparison is made with experimental data. Calculations are carried out using various potentials. It is concluded that they can be used to study the thermodynamic properties of systems including sugars, as well as their polymers, and water. The work is supported by the grant No. 18-19-00734 of the Russian Science Foundation.

Ionic conductivity of ceramics under extreme thermal loads

Savilov T M[2], Lankin A V[1,2] and Norman G E[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 141701, Russia

[@] genri.norman@gmail.com

High-temperature electrolysis of water is one of the techniques for producing hydrogen. The possibility of its implementation and efficiency are associated with the presence of ceramics with high ionic conductivity, capable of working under extreme thermal loads. Such ceramics are made on the basis of cubic zirconium dioxide. This material can remain operational up to very high temperatures, while possessing high values of ionic conductivity. This makes it important to study factors that can significantly affect this. The electrical conductivity of zirconium dioxide depends strongly on the presence and concentration of oxygen vacancies in its crystal lattice. Of great importance in the transfer of ions in such systems are crystal lattice defects associated with grain boundaries in the polycrystalline structure of ceramics. This potentially makes it possible to improve greatly the properties of such ceramics by changing the size of the grains forming its structure and introducing alloying additives. The molecular dynamics method has found wide application in the description of systems including metal oxides. In this paper, we use it to study the effect of grain size in polycrystalline cubic zirconium dioxide on its ionic conductivity at various temperatures. The values of the preexponential factor and activation energy in the temperature dependence of the mobility coefficient of the oxygen ion are calculated in materials of various structures. The dependence on the grain size of the structure of the material is obtained. The work is supported by grant No. 18-19-00734 from the Russian Science Foundation.

Ion diffusion in liquid solutions

Orekhov M A[1,2,3]

[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 141701, Russia
[3] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

maksim.orekhov@phystech.edu

It is shown with theoretical and computational arguments that statistical uncertainty of diffusivity calculated in molecular dynamics depends on the simulation box size. A multiscale approach is suggested to minimize statistical uncertainty of the simulation.

The idea is that big system is cut into multiple small systems so that total number of particles in small systems will be the same as in large system. This prevents appearing of large collective flows and fluctuations associated with them. Molecular dynamics is used to describe effects of local molecular origin and hydrodynamics is taken into account using theoretical approach.

On the other hand, simulation of the large system takes into account both local processes and hydrodynamics via a full scale molecular dynamics. It is not effective in terms of a multiscale approach.

To illustrate the application of this approach, we computed the diffusion coefficients of ions in aqueous solution. The simulation with 343 water molecules and 7 ions provides high accuracy results two times faster than the simulation with 8000 molecules and 160 ions.

Limitations for Li-ion batteries application in engine cold cranking

Fedotov A A[1,@]**, Popel O S**[2]**, Kiseleva S V**[2,3] **and Tarasenko A B**[2]

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

[@] monolitk3@gmail.com

This study focuses on the use of lithium-ion batteries in cold start systems. Down-scaled test specimen of LiC_6–Li-NMC (Li-NMC—lithium nickel manganese cobalt oxide) and LiC_6–$LiFePO_4$ batteries coupled with supercapacitor module were tested in cold cranking mode. The charge currents between Li-ion battery and supercapacitor module are experimentally determined. The actual operating temperatures ranges of such batteries are determined in relation to local climate condition and compared with single Pb-acid battery. The test results showed that significant limitations exist for current value both for Pb-acid and Li-ion battery. Coupling of supercapacitor module with Li-ion battery slightly improves the situation, but does not guarantee reliable three attempts for engine cold cranking.

2. Shock Waves, Detonation and Combustion

Strong shock waves and extreme states of plasma obtained in the Russian Federal Nuclear Center—VNIIEF in experiments at pressures up to 20 TPa

Mochalov M A[@], Il'kaev R I and Erunov S V

Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia

[@] postmaster@ifv.vniief.ru

This work presents the results of studies at the Russian Federal Nuclear Center—VNIIEF (All-Russian Research Institute of Experimental Physics) of the thermophysical properties and plasma conductivity of cryogenic liquids (nitrogen, argon, krypton and xenon) and the compressibility of gaseous helium, deuterium and their mixture under shock and quasi-isentropic compression using condensed explosives in the range of pressures reaching 20 000 GPa.

The methods used to generate and diagnose states in plasma with strong interparticle interaction are shown.

On the basis of a set of experimental data, semi-empirical equations of state of the investigated substances in the pressure range reaching the submegabar range are experimentally substantiated.

Non-ideal plasma compressibility of deuterium and helium at pressures up to 20 000 GPa

Mochalov M A[@], Il'kaev R I, Erunov S V, Arinin V A, Blikov A O, Komrakov V A, Maksimkin I P, Ogorodnikov V A and Ryzhkov A V

Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia

[@] postmaster@ifv.vniief.ru

Experimental data on the compressibility of strongly non-ideal plasmas of deuterium and helium, quasi-isentropically compressed up to densities $\rho \approx 14$ g/cm^3 at pressures up to $P \approx 20$ TPa (200 Mbar) in the devices of spherical geometry are presented. The characteristics of experimental devices, methods of diagnostics and interpretations of experimental results are described.

Trajectories of metallic shells, compressing deuterium and helium plasma, were recorded by means of pulsed power sources of x-ray radiation with electrons boundary energy ≈ 60 MeV. For the first time in the experiment as additional source of x-ray radiation a high-current accelerator was applied with electrons boundary energy ≈ 12 MeV capable of examining of objects with surface densities up to 280 g/cm^2.

Plasma densities up to $\rho \approx 14$ g/cm^3 were determined by measured magnitude of shell internal radius at the moment of its stop in each experiment. Compressed plasma pressure was obtained by means of gas-dynamic calculations, taking into account real characteristics of experimental devices.

An analysis of the developed technique allows one to rely on the possibility of studying the quasi-isentropic compressibility of deuterium and helium plasma at the Russian Federal Nuclear Center—VNIIEF (All-Russian Scientific Research Institute of Experimental Physics) up to pressures $P \approx 25$ TPa.

Registration of double compression of materials using a synchrotron

Smirnov E B[1,2,@]**, Petrov D V**[1]**, Garmashev A Yu**[1]**,
Pruuel E R**[3]**, Ten K A**[3]**, Kashkarov A O**[3]**, Rubtsov I A**[3]
and Tolochko B P[4,5]

[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] South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia
[3] Lavrentyev Institute of Hydrodynamics of the Siberian Branch of the Russian
Academy of Sciences, Lavrentyev Avenue 15, Novosibirsk 630090, Russia
[4] Institute of Solid State Chemistry and Mechanochemistry of the Siberian
Branch of the Russian Academy of Sciences, Kutateladze 18, Novosibirsk
630128, Russia
[5] Budker Institute of Nuclear Physics of the Siberian Branch of the Russian
Academy of Sciences, Lavrentyev Avenue 11, Novosibirsk 630090, Russia

[@] ewgeny_smirnov@mail.ru

Compression of matter in two shock waves compared with compression in one shock wave provides a smaller change in internal energy. The states realized due to this phenomenon are observed below the Hugoniot curve, approaching the isentrope and the isotherm. This fact attributes to the value of the experiments with double compression conducted in order to study the states of matter and its equation of state under high pressures. The paper describes the setup and the results of experiments where two modes of shockwave collision were implemented. Synchrotron radiation was used to register the processes of incident shock wave propagation and collision, as well as reflected shock wave formation. The experiments on polymethylmethacrylate and magnesium were conducted using the VEPP-3 and VEPP-4 accelerator facilities of the Budker Institute of Nuclear Physics SB RAS.

Investigating of static and dynamic properties of steels

Petukhov E A[@], Smirnov E B, Klenov A I, Sidorov K S, Shistirikov M A, Yusupov D T, Zavialov Z I and Bortsov A A

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

[@] ea_petukhov@mail.ru

This work presents the results of investigation into dynamic properties of a structural material such as stainless steel made by additive fabrication (3D printing). In the investigation, split Hopkinson pressure bar system was applied. This method allows for testing a wide range of materials and studying dynamic diagrams of compression and strain within the strain rates range of 10^2–10^3 s^{-1}. Specimens of stainless steel (analogous 12Kh18N10T steel) were obtained by laser sintering of metal powder (selective laser sintering) Using industrial 3D printer. 24 experiments were conducted with the specimens made from stainless steel. The impact or velocities ranged from 7 to 14 m/s. The intrinsic strain rates of the specimens where from 0.75×10^3 to 2.8×10^3 s^{-1}. The work gives "stress–strain" and "strain rate–strain" diagrams. The objective of the work is to study properties of stainless steel specimens fabricated by additive techniques. The following tasks are to be solved: determining the strength characteristics of the specimens made of additive stainless steel in the set of experiments using split Hopkins pressure bars technique; and comparing strength properties of additive stainless steel and its analogue, e.g., conventional 12Kh18N10T steel.

Stainless-steel solid and periodic-volume samples manufactured using additive technology and their high-strain-rate deformation with in 10^2–10^3 s^{-1}

Klenov A I[@], Garmashev A Yu, Smirnov E B, Petukhov E A, Shistirikov M A, Yusupov D T, Sidorov K S, Bortsov A A and Zavialov Z I

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

[@] klenov174@gmail.com

This work is devoted to the dynamic behavior of stainless steel samples using an additive process, i.e., three-dimensional printing. Samples having both the solid-uniform structure and also the volume-periodic structure are the subject of this investigation. Samples were loaded on the apparatus traditionally used in the split Hopkinson pressure bar method (SHPB-method) that allows a wide range of materials to be tested, as well as both the tensile-test diagram and the compression-test diagram to be studied within the strain rate range of 10^2–10^3 s^{-1}. Goals and objective of the effort: investigations into shock-wave properties of samples prepared by the additive technology; collection and analysis of data from a set of experiments of the SHPB-method. More than 50 experiments with stainless-steel samples were performed as a part of the study that gave us the stress–strain curves and the strain rate–strain curves within impact velocities from 7 to 14 m/s though the intrinsic strain rates ranged from 0.74×10^3 to 2.8×10^3 s^{-1}. Results obtained for samples manufactured by the additive technology were compared with those obtained for samples manufactured by the traditional technique. In addition, directions for the future research are outlined.

On the question of estimation of liquid–vapor phase transition critical point parameters of metals

Emelyanov A N[@], Shakhray D V and Kim V 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

The problem of determining the position of the boundaries of the two-phase region and the critical liquid–vapor transition point on the phase diagram of metals has long attracted the attention of physicists and is still relevant [1]. Nevertheless, the estimates of the critical point parameters for some metals obtained by different authors vary greatly [2]. In this paper, experiments were performed on the isentropic expansion of shock-compressed porous samples of copper and tungsten in flat geometry. The density of expanded metals was estimated from the experimental data obtained. The results of this density estimation for copper for different pressures in the region of the isentrope entrance into the two-phase region have a good agreement with the calculated data obtained using the one-dimensional hydrodynamic calculation and the equation of state (EOS). For tungsten, on the contrary, a strong difference between the obtained density estimate from experimental data and using hydrodynamic calculation and EOS is obtained. The detected differences in the estimates of the density of tungsten suggest that stratification occurs at the expansion of tungsten and another low-density phase is formed in addition to the main phase of the expanded tungsten. The presence of two phases of expanded tungsten after shock compression and expansion should significantly affect the evaporation process and the parameters of the critical point.

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Application of high-speed rotating mirror camera for holographic registration of high-speed processes

Turkin V N[@], Arapov Yu D, Kamenev V G, Kuzin V M and Shubin A S

Dukhov Research Institute of Automatics (VNIIA), Luganskaya 9, Moscow 115304, Russia

[@] Vturkin@vniia.net

An important goal in the study of high-speed gas-dynamic processes is to determine the parameters of microparticles arising from the propagation of a shock wave through a sample. In order to record the process and define parameters of particles, holographic techniques can be applied. As far as the process lasts several dozens of microseconds, it is needed to receive a sequence of images with interframe rate about 1 μs. In the report it is presented original method receiving sequence of holographic images which is based on using high-speed rotating mirror camera. It functions as follows. The coherent laser beam passes through a beam expander, illuminates a test chart, then the lens transform the light beam, in the Fourier plain of which a row of slits is perforated. As far as a beam waist is about several millimeters, the beam can pass through a narrow slit without losses. There is a little mirror behind every slit, which turns the beam and other lenses form an image for the digital camera. The rotating mirror camera is used to rotate the light beam with extremely high rate. When the light beam penetrates through every slit, an image is formed for digital camera behind every slit. It is presented simulation and experimental results.

Diagnostics of lead and its alloy melting by method of metallographic analysis of samples recovered after shock-wave loading and release

Malyshev A N[@], Ignatova O N, Ilyushkina N Yu, Skokov V I, Shimanov A V, Georgievskaya A B, Sokolova A S, Podurets A M, Tkachenko M A and Balandina A N

Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia

[@] postmaster@ifv.vniief.ru

We present results of investigation how C1-type lead and its alloy with antimony (2.7% in mass) are melted under shock-wave loading and release by the method of metallographic analysis. Samples made of the investigated material were placed inside a titanium capsule. They were loaded by a planar shock wave with use of an aluminum impactor, which was accelerated by high-explosive detonation products. The paper includes results of metallographic analysis of the samples in the initial state, after submission of them to thermal processing in normal conditions, and samples recovered after shock-wave loading. Traces of melting were revealed in lead after shock-wave loading by pressure of 25.6 GPa followed by release. Similar traces were revealed in the lead-antimony alloy at pressure by shock wave with ≈ 21 GPa.

Numerical simulation of spall in lead accounting for its occurrence in solid as well as liquid phases

Ignatova O N[1,@], Raevskiy V A[1], Desyatnikova M A[1] and Zocher M A[2]

[1] Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia
[2] Los Alamos National Laboratory, Los Alamos, New Mexico 87545, United States

[@] onignatova@gmail.com

In the present work, we use a model that was elaborated to control the development of damage in a wide range of load conditions with the possibility of applying to both solids and liquids. The model is termed Dynamics of Growth and Compaction in Solids and Liquids (DGC-SL). This model accounts for inertial forces, shear strength, viscosity, and surface tension in the initiation and evolution of damage. We apply the model to predictions of spall in lead. Those predictions are compared to empirical data taken from the work of Breed *et al*, lead samples were subjected to shock loading generated by the detonation of high explosive (HE). By varying the thickness of the HE layer, spall layers of varying thicknesses were produced. Spall thickness was measured using flash radiography. Important for the current work is a recognition that dependent upon the magnitude of the detonation-wave-induced loading of the samples, some of the samples spalled in a solid state, whereas others spalled in mixed-mode fashion involving regions of liquid within an otherwise solid body. Hence this set of experiments provide an ideal test for the validation of DGC-SL.

High strain rate uniaxial tension of conductive materials with the use of magnetic pulse method

Adamyan Yu E, Alekseev D I, Chernenkaya L V, Krivosheev S I[@], Magazinov S G and Manzuk M V

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

[@] ksi.mgd@gmail.com

Due to the high energy density, strong pulsed magnetic fields allow it to be used to generate pulses of controlled pressure in the range of microsecond duration. This paper presents a scheme of uniaxial tension of conductive materials with the use of magnetic pulse loading method, in which a mechanical impact on a material is formed by transmitting the magnetic pressure generated in a magnetic system consisting of a flat inductor and a conductive disk to which the test sample is attached. It is shown that in a magnetic system with an induction of 10 T and the first half-cycle duration of 50 μs, it is possible to obtain strain rates of up to 10^4 s^{-1} during uniaxial tension of a copper wire. Numerical simulation of the high strain rate tension process showed the applicability of the Johnson–Cook model for description of the experimental results. An increase of magnetic field induction in the magnetic system and a decrease in the pulse duration justify the expectation of higher strain rates in the direct tension mode.

Periodic error when processing data from a velocity interferometer system for any reflector

Kazieva T V

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

glizerogen@gmail.com

One of the most popular and accurate methods for diagnosing the movement of materials under shock wave loading is the VISAR (velocity interferometer system for any reflector) method [1]. This method allows to increase the reliability of mathematical models and improves the quality of empirical data on the strength properties of various structural materials. An analysis of the sources of errors and the limiting accuracy characteristics of the method is devoted to a whole series of analytical works [2–6]. This work is devoted to the analysis of the dynamic error that occurs when processing VISAR data with the use of traditional algorithms, and the influence of various factors on it.

As a result, when evaluating the velocity error in its composition, we can distinguish a constant component associated with the parameters of the delay line and the laser radiation source and a periodically changing part that is associated with the phase of the processed signal and the signal-to-noise value. The frequency of this error complicates the presentation of the final results, however, at the same time, it is possible to reduce the measurement error with the correct choice of the processing algorithm depending on the current phase. Averaging the phase value obtained by various algorithms also makes it possible to smooth out the influence of this source of measurement error.

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Sound velocities in lead during its dynamic loading

Pankratov D G[@], Poptsov A G and Yakunin A K

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

[@] f-d-f@mail.ru

In addition to [1], the results of measurements of sound velocities in shock-compressed lead are presented, performed at pressures from 13 to 95 GPa. In the range from 13 to 55 GPa, the measurements were performed by the photon Doppler velocimetry (PDV) method using LiF indicator windows, in the range from 40 to 95 GPa by combined the photoelectric and laser PDV methods [2] when using bromoform as the indicator liquid. Peculiarities associated with the occurrence of phase transformations (melting) in lead in the front of a shock wave are revealed.

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Features of axisymmetric convergence of a low-melting shell

Kuchko D P[@], Olkhovskiy A V and Shirobokov A E

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

[@] d.p.kuchko@vniitf.ru

The report presents the results of an experiment on axisymmetric convergence of a lead shell.

Results of registration of light phenomena in a shock-loaded quartz single crystal

Bazarov Yu B[1,@]**, Karpov M A**[1]**, Khaldeev E V**[1]**,
Pronin D A**[1]**, Bazarov M Yu**[2]**, Borisenok V A**[2]**,
Simakov V G**[1,2]**, Bragunets V A**[1] **and Shestakov E E**[1]

[1] Federal State Unitary Enterprise "Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics", Mira Avenue 37, Sarov, Nizhniy Novgorod Region 607188, Russia
[2] Sarov Institute of Physics and Technology of the National Research Nuclear University Moscow Engineering Physics Institute, Dukhova Street 6, Sarov, Nizhny Novgorod Region 607186, Russia

[@] yubusilver@gmail.com

The report presents the results of applying the high-speed photographic method to study the light effects in x-cut samples of a quartz single crystal when loaded with a plane shock wave with a front pressure of 1.7–1.8 GPa. It is shown that immediately after the shock wave enters the sample, local foci of light appear in it, the density of which increases as the shock wave propagates through the sample.

Experimental study of shock-wave compressiblility of docosane and paraffin

Zubareva A N[@], Sosikov V A and Utkin A V

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

[@] zan@ficp.ac.ru

The work presents an experimental study of the shock-wave properties and the structure of the front of compression pulses of docosane and homogenized paraffin in the area of low (about 0.1 GPa) and high (about 10 GPa) pressures. Paraffin is a mixture of molecules of saturated hydrocarbons from C_{18} to C_{35} ($\rho_0 = 0.91$ g/cc), while docosane is a saturated hydrocarbon $C_{22}H_{46}$ ($\rho_0 = 0.94$ g/cc).

The velocity profiles were measured with VISAR laser Doppler interferometer.

Processing of experimental data resulted in developing Hugoniots for the samples under study.

The most interesting result obtained during the experiments with docosane is the formation of a two-wave configuration (not observed only under maximum pressure). Before the shock-wave front there is a precursor. The precursor appears due to the elastic-plastic properties of docosane, and the first wave is elastic. The elastic nature of the first wave brings about the high sound speed (2.6 km/s). Paraffin has no elastic properties, and the sound speed is 1.46 km/s. When the thickness of the docosane sample is increased, the duration of the elastic precursor increases, too. Unexpectedly, the plastic wave front becomes wider at the same time. Similar blurring of the compression pulse front is typical of media with anomalous compressibility, where rarefaction shock waves are formed, and compression waves are isentropic.

To demonstrate that phenomenon, the propagation of compression waves in docosane is compared to that of fused quartz, the anomalous compressibility of which is well-known.

Explosive schemes for gas-dynamic technologies of strength tests of constructions

Ostrik A V, Nikolaev D N and Cheprunov A A[@]

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

[@] alexander.cheprunov@yandex.ru

Gas-dynamic technologies are widely used in strength tests of flight vehicles [1–3]. The current trend of development of this technology is the use of low impulse explosive generators of microsecond pressure pulse duration and providing highly simultaneous loading of the constructions. Analysis of known explosive schemes is presented in the work. Prospects for the development of these schemes are discussed. The following explosive schemes are considered: cellular or sheet contact-sector scheme; tape and sheet scheme; shell and channel scheme. The most promising are tape scheme and shell-channel scheme with controlled initiation. The considered explosive schemes are used for strength tests of thin-wall constructions when the action of the directed energy fluxes of various physical nature [4] takes place.

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Pneumatic projectile launcher for low-speed strength tests of constructions to impact of bodies

Ostrik A V[1], Nikolaev D N[1] and Bakulin V N[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 Applied Mechanics of the Russian Academy of Sciences, Leninsky Avenue 32a, Moscow 117334, Russia

[@] vbak@yandex.ru

During operation, aircraft structures may be subject to low-speed exposure to solids (bullets, debris, soil particles, birds, etc). Despite the relatively low speed (up to 1 km/s), their kinetic energy is of the order of MJ for a body weight of up to several kilograms and represents a serious danger to the strength of composite constructions.

The pneumatic projectile launcher was designed and verified for strength tests on the action of low-speed bodies impact. The projectile acceleration system with an additional receiver camera and two membranes gives the compact body a speed of up to 700 m/s when its weight is up to 200 g. The device allows operation at substantially accurate pressure in the main receiver which provides the high stability of the speed of projectile. Note that the velocity stability does not depends on the accuracy of the diaphragm manufacturing. The projectile velocity measurement system is based on its passage through four wire barriers. Resistance–capacitance circuits are activated when the body overcomes barriers. Signals from the chains are recorded by a four-channel oscilloscope in the form of steps. The data obtained during the experiment allow to interpolate the x–t dependence with 4 points and find the velocity of the projectile with accuracy better than 1%.

In further work, the tests on mechanical response strength of cylindrical shells made of high-modulus composite materials on low-speed impact are planned.

Unified stand for modeling the combined thermal and mechanical action of energy fluxes on aircraft constructions

Ostrik A V, Nikolaev D N, Bugay I V[@] and Cheprunov A A

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

[@] irinbug@yandex.ru

The development of technologies for modeling the combined thermal and mechanical action of energy fluxes of different physical nature on flight vehicles is practical and important task of applied physics [1,2]. Sets of devices for modeling thermal and mechanical action of radiation and particle fluxes (RPF) are verified and widely used [1]. But their joint use requires the development of special unified stands. A new unified stand allowing to investigate the joint thermal and mechanical action of RPF on the aircraft constructions with simultaneous simulation of flight conditions is proposed. Modern means of rapid heating of structures (with the help of contact current-conducting plate, sheet pyrotechnic charges and microwave emitters of high power—magnetrons) are used. Temperature profiles realized in practice can be obtained by means of various combinations of heating means of external and internal sides of the construction. Note that magnetrons have not previously been used in strength tests for combined thermal and mechanical effects of RPF.

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Atomistic simulation of shock-wave experiments on isentropic expansion of aluminum into air

Markina E M[1,2,@], Fokin V B[1] and Levashov P R[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 141701, Russia

[@] lenmarkina@gmail.com

Experiments on the isentropic expansion of metals previously compressed by a shock wave into different anvils provide unique information on the properties of a liquid and a plasma at supercritical parameters. However, theoretical interpretation of such experiments is difficult and requires the knowledge of an equation of state. Expansion into a gas from high-pressure initial states usually occurs faster than predicted by theoretical analysis. One of possible explanations of this discrepancy is the formation of jets on the rough surface of the sample when the shock wave reaches this surface. In this work we present the results of molecular dynamics simulation of shock-wave compression and subsequent isentropic expansion of aluminum into gas at different pressures. Various shock-wave velocities in aluminum were investigated, including corresponding to the experiment [1]; cases with ideal and rough surfaces were also considered. We discuss the influence of modeling parameters on the results, including interaction potential effects.

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Nucleation of cubic ice during dynamic compression of liquid water: Molecular dynamics study

Nikolskiy V P[1,2] and Stegailov V V[1,2,3,@]

[1] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

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

[3] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] stegailov@gmail.com

Experiments on multiple compression by a shock wave revealed rapid freezing of water compressed above 2 GPa [1]. Later it was shown that the mechanisms of this transition include both heterogeneous and homogeneous nucleation processes [2]. The pressure wave profiles above 5–6 GPa have been explained recently using the classical nucleation theory [3]. However, some specific assumptions have been used, e.g., the assumption of liquid and solid co-existing at different temperatures. Valuable insights into the nature of ice nucleation process can be expected from molecular-dynamics (MD) simulations. There are system size and time length limitations for MD calculations with interatomic models appropriate for liquid–ice transition studies (TIP4P). These limitations can be overcome with the new graphics-processing-unit algorithm for TIP4P model implemented in LAMMPS recently [4]. In this report we present the first results of the large-scale MD simulations of ice nucleation during dynamic compression that have been obtained using this computational tool.

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Propagation and attenuation of shock waves in solid heterogeneous media

Kolotilov V A

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

kolotilov1992@gmail.com

In this work, a numerical study of the propagation of shock waves in a solid medium by the finite difference method CABARET [1] is performed. A good localization of shock waves was demonstrated. The verification of the method is shown by the example of the Riemann problem [2]. Shock Hugoniot line was constructed numerically for the example of a homogeneous and two-component medium, which is being constructed at each instant of time. The shock adiabat obtained as a result of averaging by the mixtures of the medium and taking into account each of the two phases directly in solving the system of non-isentropic hydrodynamic conservation laws was compared [3].

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Numerical simulation of the interaction of the shock wave with a forest

Klinacheva N L

South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia

klinachevanl@susu.ru

When cosmic bodies fall on the earth as a result of their deceleration in the atmosphere, air shock waves arise. Their destructive effect is determined by the pressure jump at the front, the duration of the compression and rarefaction phases, and the gas velocity behind the front. Bodies ranging in size from 20 to 100 m are braked at heights from several kilometers to 20–30 km. In this case, the shock waves reach the surface, causing significant damage (as, for example, when the Tunguska cosmic body falls) [1]. The construction of models that adequately describe the destructive effect of such shock waves will allow us to evaluate the possible consequences of the fall of large meteoroid bodies on Earth.

In this paper, the interaction of spherical shock waves with coniferous forest is numerically investigated. It was taken into account that when the threshold value of the pressure head is exceeded, the pine needles break off. When constructing the model, empirical estimates of vegetation parameters presented in the literature were used [2,3]. A system of differential Euler equations in cylindrical coordinates and equations describing the force interaction of gas and solid particles were chosen as a mathematical model describing the processes under study [4].

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Metastable shock waves in the region of their ambiguous representation

Konyukhov A V[@], Levashov P R 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 behaviour of shock waves belonging to the Hugoniot sections adjacent to the region of the shock wave instability $L > 1 + 2M$ [1] from the side of greater and lower pressure is considered. Modified model equation of state [2] is used. The parametric study with varying shock wave parameters in two- and three-dimensional formulations is performed. It is shown that the shock waves belonging to the Hugoniot sections with ambiguous representation of the shock-wave discontinuity are metastable. The perturbed shock waves go into oscillating mode at large amplitude of the perturbation. Otherwise the behavior that is characteristic for neutrally stable waves is observed: weak damping of secondary waves with the sound emission by the shock wave surface. This is explained by the fact that the neutral stability condition [3] is fulfilled in the segment of an ambiguous representation of the shock-wave discontinuity. The averaged characteristics of the shock wave in the oscillating mode are calculated and analyzed.

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Analysis of wave phenomena in hot nuclear matter in the presence of critical point of quark-hadron phase transition

Konyukhov A V[@], Levashov P R 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

In media with a first-order phase transition, instead of a single compression shock wave and an isentropic rarefaction wave, a composite wave configurations can occur, including, along with the usual elements, isentropic compression waves, rarefaction shock waves and sections of constant parameters [1]. In this paper, an attempt is made to analyze the relationship between the presence of the critical point of the quark-hadron phase transition and the emerging composite wave structure. The analysis is performed on the basis of a model equation of state of hot nuclear matter with a critical point of the quark-hadron phase transition, constructed using the model of hadron gas with repulsion of particles and the "bags" model. The model equation of state qualitatively describes the smooth change of thermodynamic properties observed in lattice QCD (quantum chromodynamics) calculations in the crossover region, and the jump corresponding to the first-order phase transition in the region of large values of the baryon chemical potential [2]. Taub shock adiabats and Poisson adiabats crossing the crossover region and the first-order phase transition region in the vicinity of the critical point are constructed. The results of calculations show the formation of an isentropic wave in the structure of a composite compression wave when passing through a critical point. The work is supported by the Research Program No. 6 of the Presidium of the Russian Academy of Science.

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New deflections for the flow of Prandtl–Meyer

Ferreyra R T and Gongora J G[@]

National University of Cordoba, Avenue Velez Sarsfield 1611, Cordoba X5000, Argentina

[@] ricardotf45@hotmail.com

A new formulation by components for the deflection of the Prandtl–Meyer flow is obtained. For this purpose, the radial and transverse components of the deflection of the flow are recognized through a geometric analysis. According to the specialized literature, the deflection can be obtained by an exact analytical method by integrating from an initial state (incident flow) and arriving to the pre-established final state (deflected flow) [1–3]. So, the integration region is the same expansion region. In the same sense, the deflections associated with numerous intermediate states can be achieved by computational progress advancing from one limit state to the other one. The aim of this work is to provide relative access to the infinite intermediate states in analytical, exact, selective and by components [4–6]. The contribution in the field of computational fluid dynamics is to facilitate the analysis of the Prandtl–Meyer flow to access to an arbitrary number of deflections.

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Some peculiarities of strain localization and failure in condensed matter under shock compression

Bayandin Yu 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

The object of mathematical modeling is condensed matter with defects like micropores, microcracks, and microshears. The purpose of the present research consists in the explanation of mechanisms of structural relaxation of stresses and failure in condensed matter with defects based on the analysis of the multiscale collective behavior of mesoscopic defects. The studies relate to fundamental aspects of the mechanisms of strain localization and fracture in condensed matter in a wide range of strain rates and are aimed at developing the constitutive relations (equations of state) when compared with the results of dynamic and shock-wave experiments, verification of the developed models of the behavior of solids and liquids under dynamic and moderate-shock loading intensities using original experimental techniques and developed mathematical models adapted to commercial software packages.

The mechanisms of structural relaxation and fracture in solids caused by the multiscale collective behavior of mesoscopic defect ensembles and self-similar laws of plasticity and fracture development have been experimentally and theoretically investigated. The mechanisms of the instability of plastic deformation and staged fracture are considered in the framework of a special type of critical behavior of condensed media with mesoscopic defects—structural-scaling transitions, linked with the evolution of collective modes of mesoscopic defects. These collective modes are of the nature of self-similar solutions for the damage kinetics (auto-solitary waves), playing the role of collective variables assigning with the spatio-temporal dynamics behavior of condensed matter under impact loading.

Thermomechanical properties of the aluminum–magnesium alloy in the wide range of strain rates: Model and experiment

Uvarov S V[@], Bayandin Yu V, Naimark O B and Bilalov D A

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

The constitutive model for thermomechanical properties of alloy of aluminum and magnesium for the broad strain rate conditions is presented. As it mentioned in [1] the study of the efficiency of the thermomechanical conversion, expressed as the Taylor–Quinney coefficient reveals a new correlation between the thermomechanical characteristics of a material and its deformation micromechanisms, that should find its way into constitutive models. This model is a further development of the statistically based approach developed by Naimark [2] with the addition of the thermal coupling. The proposed model previously was used to study the process of fatigue failure of a structural alloy AlMg2.5 [3]. The model parameters were identified and verified using experimental data on static, dynamic and fatigue loading, as well as tests at various temperatures. Data were obtained from the literature and from our own experiments. The verification experiments were carried out. In the modified Taylor tests the contact force and the temperature field dynamics were recorded and then compared with the numerical simulation.

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The calculation of the optimal corrugation of the plate during explosive welding

Shutov A V[@] and Sultanov V G

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

Explosion welding is performed by oblique collision of the plates at a certain angle α_c, when the speed of the contact point with the plates parallel to each other is equal to the detonation velocity D_{exp}, which, in turn, is usually lower than the speed of sound at welded materials. In [1] it was shown that for a given collision velocity of plates, there is an optimal collision angle α_{opt}, at which the maximum compression and heating on the contact line of these plates is achieved. The speed of the contact point, in this case, is equal to the speed of the shock wave propagating along the contact D_{opt}. In the presented work, it is proposed to use a special corrugation of one of the plates like a saw with a triangular teeth to achieve that on the front slope of the tooth, the plates contact at an angle α_{opt} with the corresponding speed of the contact point D_{opt}, while the average speed of the contact point remains D_{exp}.

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Features of shock compression wave propagation in a medium with a given porosity

Ziborov V S[@] and Rostilov T A

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

[@] ziborov.vs@yandex.ru

The method of laser interferometry is used for measuring the structure of the shock compression wave in media with a given porosity in the region of existence of a two-wave configuration. Velocity profiles of the free surface of samples from an epoxy compound containing hollow glass microspheres in the ratio of 1/1 and 1/3 volume fractions, in the range of shock compression pressures of 0.3–1.1 GPa, were obtained. The dependence of the maximum velocity gradient of the primary wave front on the impact compression pressure for samples that differ in pore content is obtained. It was found that the velocity gradient is significantly greater in samples with a lower content of hollow microspheres, the difference decreases with increasing compression pressure, and disappears at $P \geqslant 1$ GPa. The dependence of the maximum velocity gradient of the primary wave front on the impact compression pressure for samples that differ in pore content is obtained. The power indicators of the dependence of the largest gradient of the front velocity for the primary and main waves are determined.

Simulation of shock wave propagation in a porous medium of nickel nanoparticles

Fokin V B[@], 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

[@] Vladimir.Fokin@phystech.edu

A porous medium of micro- and nanoparticles of various sizes has a lot of interesting physical and chemical properties useful for a wide range of applications in science and technology (in particular, to obtain refractory substances, as reaction mixtures with controlled burning rate, in ammunition, in space technology and in medicine). In this work, we study a system of nickel nanoparticles with sizes up to about 50 nm. To produce a sample consisting of nanoparticles a special procedure has been worked out. The propagation of shock waves with different velocities through a nanoporous sample is calculated using classical molecular dynamics, and the results are compared with the simplified Zeldovich's model [1]. The shock Hugoniot curve thus obtained can be directly measured experimentally that allows a direct verification of simulation data.

We investigate the influence of the sample porosity, the concentration of nanoparticles, and also various types of sample defects on the the process of shock wave propagation and parameters of shocked matter.

Classical atomistic simulation also allows one to study surface effects in a nanoporous material, as well as processes occurring at the interface between reacting nanoparticles.

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Experimental study of shock wave reflection from perforated plates

Mikushkin A Yu[1,2,@], Golub V V[1], Zhilin Yu V[1], Cherpakova A A[1] and Bocharnikov V M[1]

[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

[@] mikushkin-anton@yandex.ru

Many experimental and theoretical papers have been devoted to the study of the interaction of shock waves with permeable obstacles, for example, [1, 2]. This is primarily due to the practical tasks of protecting against the destructive impact of shock waves on various structures and technological equipment. This paper presents the results of experimental studies of shock waves reflected from perforated plates of different permeability. The results of measuring the Mach number of the shock wave reflected from single plates as a function of the Mach number of the primary wave are presented. Based on the results of the experiments, the approximation dependence of the Mach number of single shock waves reflected from the plates on the Mach number of shock waves reflected from the solid end is proposed. The results of measuring the Mach number of shock waves reflected from different packages of plates are also presented.

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Atomic resonance absorption spectroscopy study of reaction of dimethyl ether with oxygen behind shock waves

Bystrov N S[1,@], Eremin A V[1], Emelianov 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

[@] bystrovns.jiht@gmail.com

Dimethyl ether (DME) is a promising substitute for diesel fuel. Significant resources have been spent on the development of a chemical kinetic mechanism of combustion of this biofuel. The main objective of this research was the experimental study of the interaction between DME and O_2 at the high temperatures. The kinetics of reaction of DME with N_2O behind reflected shock waves is studied. The quantitative measurements of the time profiles of the concentration of oxygen atoms in the ground electronic state $O(^3P)$ were first carried out by the precisive method of atomic resonance absorption spectroscopy (ARAS) on a resonance vacuum-uv line of an oxygen atom at 130.5 nm. An experimental study of the appearance and consumption of oxygen atoms during the reaction of DME with O_2 in mixture 10 ppm N_2O (10–1) ppm DME in Ar was performed. Along with experimental measurements, a detailed kinetic analysis was carried out using the Chemkin package, consisting of a simulation of the DME oxidation process using existing kinetic mechanisms and a corresponding sensitivity analysis of the reactions under consideration. The data obtained in the course of a comprehensive study provide new valuable information on the features of the interaction of DME with O_2 at high temperatures. The support of this study by grant No. 18-38-20085 from the Russian Foundation for Basic Research is gratefully acknowledged.

Dependence of the evaporation temperature of iron nanoparticles on their size

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 dependence of the properties of iron nanoparticles on their size is investigated. The iron nanoparticles were formed in the pulse uv laser photolysis of $Fe(CO)_5$ vapor in argon atmosphere. An additional pulse ir-laser heating of formed nanoparticles at different times from the moment of its formation allowed measuring particle size and particle evaporation temperature by laser-induced incandescence technique. Simultaneous application of the time-resolved laser-induced incandescence and the laser light extinction techniques provided an observation of the particle evaporation process caused by laser heating. The particle evaporation temperatures were found to be in the range of 2100–2600 K in dependence on particle size and pressure of bath gas. The known size dependent equations of nanoparticle evaporation temperature were examined by comparison with obtained experimental data.

The detonation initiation in the combustible mixture with the particle suspended in the flow behind strong shock wave front

Efremov V P and Obruchkova L R[@]

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

[@] o_liliya@ihed.ras.ru

On the shock impact with the motionless particle suspended in the flow the local gas characteristics in the vicinity of the particle are changed. An assumption was made that the energy transformation is sufficient to initiate the detonation. The suggestion of explosion hazardous role of single particle was examined in work [1]. In work [2] our investigation was further developed and heat-generating chemical reactions were added. In work [3] detonation limits were obtained for different concentration rates.

This work is devoted to the verification of energy transformations in a gas stream due to phenomena of various physical nature. There are two phenomena causing release of heat. First phenomenon is stopping of the inert gas on the particle and another one is temperature increase as a result of exothermic chemical reactions. There is counteracting heat absorption from gas mixture into the solid particle. In present work the energy fractions related to each phenomenon were compared. It also was observed good agreement between the analytical evaluation and simulation of propagation of total released heat into solid sphere.

The spatial and temporal ranges of used methods validity are discussed.

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Nonequilibrium excitation of $a^3\Pi_r$ state of CO in oxidation reactions behind shock waves

Bystrov N S[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

[@] aemelia@ihed.ras.ru

The study of exothermic reactions during the combustion of organic fuels is of primary importance in chemical kinetics.The various kinetic schemes elaborated for modeling of the oxidation of hydrocarbons in the high temperature range do not consider the possible excited states of molecules that can affect combustion processes at certain time intervals. The CO molecule is of particular interest, since at high temperatures it can potentially activate new reaction pathways, or influence existing branching ratios, which leads to a redistribution of the composition of the products. Therefore, in this work, an experimental study of the appearance of an electronically excited state of carbon monoxide CO ($a^3\Pi_r$), which is formed in reaction processes behind shock waves, was carried out. The experiments were performed in mixtures of CH_4 with N_2O and O_2 in argon at temperatures of 2200–3500 K and pressures of 2.4 ± 0.4 bar. Peaks of nonequilibrium uv radiation from the Cameron bands of the CO molecule at a wavelength of 216 nm, which sharply increases with increasing temperature, were recorded. Simultaneously with the CO emission signals, an absorption of atomic oxygen was monitored by atomic resonance absorption spectroscopy (ARAS) at a wavelength of 130.5 nm. To quantitatively determine the concentration of electronically excited state of CO, a series of calibration experiments was carried out in mixtures of 5% and 10% CO in argon at temperatures of 4000–5000 K. The support of this study by grant No. 18-38-20085 of the Russian Foundation for Basic Research and a program of the Presidium RAS is gratefully acknowledged.

Experimental measurements of $CO(a^3\Pi_r)$ and $O(^3P)$ concentration profiles at high temperature oxidation of biofuels

Bystrov N S[1], Emelianov A V[1], Eremin A V[1], Loukhovitski B I[1,2], Sharipov A S[1,2] and Yatsenko P I[1,3,@]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Central Institute of Aviation Motors, Aviamotornaya Street 2, Moscow 111116, Russia
[3] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] pavelyatcenko@yandex.ru

An experimental study of $CO(a^3\Pi_r)$ and $O(^3P)$ concentration profiles at oxidation of biofuels, such as dimethyl ether and n-butanol was carried out in a wide temperature range from 1890 to 3250 K at pressure of 2.4 ± 0.4 bar using emission and absorption spectroscopy. In all investigated conditions, the peaks of nonequilibrium uv radiation of electronically excited carbon monoxide $CO(a^3\Pi_r)$ were observed. Besides, the resonant absorption profiles of atomic oxygen in the ground electronic state $O(^3P)$ converted to O-atom concentration profiles were for the first time measured at this temperature range. For simulating the $CO(a^3\Pi_r)$ radiation experimental profiles a kinetic mechanism of its formation and consumption was developed. This mechanism was implemented into the existing comprehensive detailed kinetic models, which were then tested on the obtained experimental profiles of atomic oxygen and electronically excited carbon monoxide. It was shown that the proposed $CO(a^3\Pi_r)$ sub-mechanism nearly correct describes the ongoing reaction processes, however, complete compliance was not achieved. To elucidate reactions responsible for the differences observed, the sensitivity analysis was performed. This work has been supported by grant No. 18-38-20085 of the Russian Foundation for Basic Research.

Environmentally friendly energy cycle using carbon condensation energy

Eremin A V 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

Several years ago, the authors comprehensively studied the formation of the detonation condensation wave that occurs during the self-decomposition of acetylene behind the shock wave [1, 2]. Later, the authors proposed to use this effect to create an environmentally friendly anaerobic power engine operating on acetylene [3]. Another, more general approach to creating an environmentally friendly energy cycle is the development of devices that use fossil fuels. Therefore, if the purpose of the elaborating energy cycle is not to develop an anaerobic acetylene-powered power engine (as suggested in [3]), then there is no need for a very energy-consuming process for the direct production of acetylene from methane. Thus, the most efficient use of carbon condensation energy would be in the direct pyrolysis of methane with the formation of hydrogen and carbon vapor. In this work, we present a schematic diagram of a circular cycle with the pyrolysis of methane to hydrogen and soot and following combustion of the generated hydrogen for the heating of initial methane up to pyrolysis temperatures and estimations of the energy parameters of such a process.

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The dynamics of carbon structures during the detonation of benzotrifuroxan

Satonkina N P[@] and Ershov A P

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

[@] snp@hydro.nsc.ru

Benzotrifuroxane (BTF, $C_6N_6O_6$) is one of the most powerful explosives with a number of interesting features. This is an anhydrous explosive substance, in the detonation products of which structures of record size have been found. Previously, it was customary to explain this fact by the high temperature, due to which the state of the carbon in the phase diagram corresponded to the liquid phase. But, as shown in work [1], BTF is not outstanding for this characteristic. In work [2], the conductivity during BTF detonation was investigated, and it was shown that the conductivity profile is also qualitatively close to those obtained for high-power explosives. In work [3], it was suggested that the large size of nanodiamonds in BTF detonation products is associated with the absence of hydrogen in the BTF molecule.

Since conductivity is determined by carbon, it is possible to diagnose condensation and the formation of carbon structures by electrical conductivity, which is done in this work.

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Investigation into detonation propagation in cylindrical samples of triaminotrinitrobenzene-based explosive compositions

Galiullin I G[@], Sarafannikov A V, Dunayev V N, Gagarkin D M, Dudnik D P, Shahmayev S V and Salahov I F

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

[@] galiullin-igor@mail.ru

This paper presents experimental studies of velocity and shape of the detonation wave front that propagates in cylindrical samples of explosive compositions based on triaminotrinitrobenzene (TATB), fabricated according to two different techniques: chloranilic one used 2,4,6-trichloraniline and phloroglucinol one used 1,3,5-phloroglucine. Fluoropolymer served as a binder in all explosive compositions. Detonation velocity and front shape were investigated on cylindrical samples with the diameter of 60 mm. The samples were initiated by the diverging detonation wave. Detonation velocity of explosive compositions was investigated using the electrical contact technique. Streak camera with linear slot sweep recorded time profiles of detonation wave arrival at the sample end surface, and then these profiles were recalculated into the shape of the detonation front with regard to recorded detonation velocities. As a result, this work allowed us to estimate the influence of TATB synthesis technology on the velocity of the steady detonation and curvature of the detonation front for explosive compositions under study.

Mach reflection in detonation front interaction with shock-wave lens

Sultanov V G[@], Zaitsev V Yu, 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

[@] sultan@ficp.ac.ru

The work describes an interesting and practically important feature of the behavior of the detonation front near the shock-wave lens surface—the transition from regular mode of reflection to irregular, namely Mach reflection. This feature has a significant impact on the shock wave front geometry before and after the lens and should be taken into account when constructing such lenses. The work was carried out as part of the experiments to obtain axisymmetric cylindrical convergent detonation front at the multipoint initiation (18 points, main charge diameter 200 mm). The symmetry of the shock wave output for the lens constructed by the authors on the surface of the main charge was studied. The cylindrical shock wave at the lens exit was obtained at 14.5-mm width (of 35-mm lens). The impossibility to obtain a wider (full width of the lens) cylindrical front is explained by the transition from regular to Mach reflection moving along the lens surface in the initiating socket of the detonation front.

Kinetics and products of fast-flowing reactions in the CuO–Al nanothermic system

Badretdinova L Kh[1,@], Stankevich A V[1,2], Bakirov A R[2], Valiev R N[1] and Bazotov V Ya[1]

[1] Kazan National Research Technological University, Karl Marx Street 68, Kazan, Republic of Tatarstan 420015, 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

[@] badretdinova_kstu@mail.ru

With the development of modern industry and nanotechnology, new composite energy materials, nanothermites, have recently become widespread, the chemical interaction between the components of which proceeds much faster than in classical termites [1] and approaches explosive.

In this work, the influence of the initial chemical composition and structure of CuO–Al nanothermites on the kinetics of the fast-flowing reaction of the interaction of components, the chemical composition and flash delay under quasi-isothermal action is studied. The initial samples were presented both in the nanodispersed state (powders) and in the form of multilayer thin films. It is shown that at reaction rates above 300 m/s aluminum oxides of different stoichiometric composition Al_xO_y and copper are formed, and at speeds less than 500 cm/s various aluminum hydroxide compounds, copper oxides and spinel-type intermediates ($Al_xCu_yO_z$) are formed.

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Ignition of nanothermites by laser impulse

Grishin L I[1,2], Dolgoborodov A Yu[1,2,3,@], Kirilenko V G[3] and Brazhnikov M A[3]

[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] Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, Kosygina Street 4, Moscow 119991, Russia

[@] lenya-grishin@mail.ru

Ignition and flame propagation in nanosized thermite mixtures Al–CuO and Al–Bi_2O_3 caused by laser pulse radiation were studied. Nanothermites were manufactured with the use of ultrasonic mixer were tested. The samples were ignited by laser with wavelength 808 nm and average power of 3.5 W. For the termites, using two-channel pyrometer, there were measured minimum ignition energy and average burning velocity as a function of sample porosity. The effect of compounds aging on the sensitivity to the laser pulse was studied. The results showed a strong dependence of the burning rate and initiation energy on the porosity of the samples. On the basis of the obtained results, there were put forward the assumptions on the mechanism of the reaction of combustion in nanothermites exposed to laser radiation, in particular, the assumptions in two stages of the reaction. Ignition delays, combustion rates and laser initiation energy were experimentally measured for Al–Bi_2O_3–F_{42} and Al–CuO. For the Al–CuO composition, the effect of "aging" on the results of initiation and propagation of the reaction under the influence of a laser pulse was determined for the first time.

The study of the combustion wave of linear charges from mechanically activated thermite mixtures

Ananev S Yu[1,@], Grishin L I[1], Yankovsky B D[1] and Dolgoborodov A Yu[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, Kosygina Street 4, Moscow 119991, Russia

[@] serg.ananev@gmail.com

The burning of termite mixtures is usually represented in the form of a wave. In this case, the geometric coordinate is taken as the wave front, where the value of the measured parameter reaches a given level. The burning speed of such a coordinate is taken as the burning rate. Correlation of measurement data of different parameters allows to make a detailed representation of the course of the combustion process.

In this work, the oscillograms of electric current through the reaction region between electrodes with a given potential difference, chronograms of the operation of piezoelectric sensors and photodiodes, pyrometric measurement data, and photographs of the glow region are obtained and analyzed. The most part of results were obtained using $Al+CuO$ mixtures, as well as $Al+Bi_2O_2$ ones of pour density with linear charge porosity of 50–65%. The initiation of combustion was carried out by an electric discharge ($\geqslant 0.1$ J) in a spark gap of 1 mm for 0.6 s.

Analysis of the measurement data allowed us to more accurately determine: advanced gas filtration through the mixture pores; charge generation, which ensures the electrical conductivity of the products; electron recombination, and optical radiation with an increasing density of reaction products.

Detonation properties of aqueous solution of hydrazine nitrate

Utkin A V, Mochalova V M[@], Garanin V A and Romanova L B

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

[@] roxete20000@mail.ru

The use of hydrazine nitrate (HN) as one of the components of rocket fuel requires the determination of its detonation properties, sensitivity to shock waves and critical detonation parameters. However, the available data on the detonation properties of HN are extremely limited and not always unambiguous. It is very important to know the effect of water on detonation properties of HN due to its high hygroscopicity. The purpose of this work is to determine the detonation parameters and critical concentration ratio of aqueous solution of HN. The structure of detonation waves, range of concentration of detonation propagation, detonation parameters and the dependence of detonation velocity on the water concentration were investigated by a VISAR interferometer. It is shown that the detonation velocity of aqueous solution of hydrazine nitrate decreases linearly with increasing concentration of water, whereas for pressed HN, the change of the detonation velocity with variation of the initial density is not monotonic, but has a characteristic s-shape. Experiments on the initiation of detonation under shock wave action for pressed HN samples of maximum density were performed. It was observed the low shock wave sensitivity, which was much lower than that of TNT. The limits of detonation propagation were found for HN–water solution. When the water concentration is equal to 36% and more, the solution becomes a non-detonating liquid.

Investigation of influence of continuous rotating detonation model facility flowpath shape on working process characteristics

Sidorov R S

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

rodik@myrambler.ru

Combustion of fuel in a continuously rotating detonation wave (DW) is one of the options for organizing a working process in annular combustion chambers (CCs) of promising liquid propellant rocket engines (LPREs) and airbreathing jet engines (AJEs). One of the principal differences between LPRE and AJE of this type concludes in direction of pressure leakage after DW: both up- and downstream in AJE and only downstream in LPRE. Similar situation takes place during the ground tests with connected air manifold of detonation CC with shaped aerodynamical nozzle with smooth generatrix and with sudden widening. It is shown in this paper during two- and three-dimensional numerical simulation that for working process realization the pressure of oncoming flow can be lower in CC with sudden widening. Also the special boundary condition placing a wall along a higher pressure zone after DW can be quite correctly used. Central body shape influence is analyzed as well.

Laser-induced fluorescence for diagnostics of polyaromatic hydrocarbons formed in pyrolysis of hydrocarbons behind shock waves

Drakon A V, Eremin A V, Korshunova M R[@] **and Mikheyeva E Yu**

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

[@] ekaterina.mikheyeva@gmail.com

The mechanisms of polyaromatic hydrocarbons (PAHs) growth were actively developed as a part of soot formation kinetics recently [1]. Laser-induced fluorescence (LIF) is promising *in situ* diagnostic for detection of PAHs in flames [2]. In this work, for the first time, the LIF was used to monitor the growth of PAHs formed during the pyrolysis of hydrocarbons behind shock waves. The PAHs fluorescence was excited using an Nd:YAG laser at a wavelength of 266 nm. The fluorescence spectrum was recorded using an ACTON SP150 monochromator and an Andor iStar optical ICCD (intensified charge-coupled device) camera. The temperature dependences of the evolution of the total spectral fluorescence signal from growing PAHs for different reaction times from the onset of the pyrolysis process were obtained. The key PAHs including benzene (one ring), naphthalene (two rings), anthrocene (three rings) and pyrene (four rings) according to the spectral dependence of the fluorescence intensity were identified. Kinetic modeling of PAHs and soot formation for experimentally studied conditions was carried out. It was shown that large PAHs consisting of four or more aromatic rings are precursors for the appearance of a condensed phase, and are probable nuclei of carbon nanoparticles. This work was supported by the Russian Foundation for Basic Research (grant No. 18-38-20085).

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The effect of gas density in metal tube cavity inside high-explosive detonating charge on the formation of cumulative jet

Sokolov M A[@], Dolgikh S M and Smirnov V N

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

[@] sokolovm1982@mail.ru

We experimentally investigated the effect of the initial gas density on the prevention of dust-like jet formation in the gas inlet pipe. The following parameters were varied: tube material (copper and steel); tube diameter (3 and 6 mm); and gas type (argon, helium) imitating deuterium–tritium gas in density. Models of planar geometry were used in the experiments. The outlet of cumulative jet from the tube and the arrival of detonation wave onto the high-explosive surface matched with the tube flange were recorded using electrical contact and optical techniques. The advance of cumulative jet in the tube relatively to the detonation wave was measured versus gas density. The dependence of the advance on gas density in the tube which was found out to be a falling exponent was obtained. The results obtained agree with the data obtained beforehand using gas imitators made of solid materials (polyurethane foam, cotton, and foam plastic).

Optical properties of flame soot and their correlation with internal structure of nanoparticles

Kolotushkin R N[1,2,@], Gurentsov E V[1] and Eremin A V[1]

[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

[@] kolotushkin.roman@gmail.com

In this study, we measured the absolute value of the refractive index functions of soot nanoparticles $E(m, \lambda)$ at wavelength $\lambda = 1064$ nm and the ratio of the refractive index functions at two laser wavelengths of 532 and 1064 nm in a premixed ethylene–air flame and acetylene–air flame by laser induced incandescence. The value of $E(m, 1064 \text{ nm})$ as well as the ratio $E(m, 1064 \text{ nm})/E(m, 532 \text{ nm})$ increased with flame height. These changes were attributed to the process of soot particle growth and structure transformation. The samples of soot nanoparticles were analyzed using high resolution transmission electron microscope (HR TEM). The procedure of HR TEM image analysis involves the separate steps of allocation of a characteristic section of the soot structure on HR TEM image, fast Fourier transformation of image, filtering, reverse Fourier transformation, binary image conversion, skeletonization and quantitative analysis of fringes structure. In dependence on height above a burner (HAB) the differences in soot structure were investigated. The collected soot particles were found to be in amorphous phase with large distances between graphene-like layers (0.5–0.55 nm) in opposite to graphite structure (0.335 nm). The main difference between soot nanoparticles observed at different HABs consisted in different size of graphene-like planes increased from 1 up to 1.2 nm at HAB increase from 10 to 20 mm. The obtained data provided the comprehensive information on the optical properties of soot in premixed ethylene–air and acetylene–air flame in dependence on HAB. The reported study was funded by Russian Science Foundation, project No. 19-79-10204.

Buoyant flames in near the lower flammability limit hydrogen–air mixtures

Gavrikov A I[1,2,3,@]**, Golub V V**[2]**, Volodin V V**[2]**, Danilin A**[3] **and Mikushkin A Yu**[2,4]

[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
[3] Nuclear Safety Institute of the Russia Academy of Sciences, Bolshaya Tulskaya Street 52, Moscow 115191, Russia
[4] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] gavrikovandrey@yandex.ru

This paper presents results of large-scale experiments and numerical simulations of premixed near the lower flammability limit hydrogen–air spherical flame propagation. Experiments were carried out in a cylindrical volume of 4.5 m^3 covered with thin polyethylene film. The effect of buoyancy and stability of the flame ball in unconfined volume are studied experimentally and numerically. Numerical analysis of the problem shows that the flame ball becomes unstable after some period of stable propagation that qualitatively corresponds with experimental results. The effect of chemistry in a flame ball propagation process is studied numerically. Comparison of experimental results and numerical simulations is presented. Comparison of numerical simulations with and without chemistry is shown. The subject and results of the study are crucial for the industrial explosion safety and hydrogen safety of nuclear power plants.

Impact of methyl radical additives on kinetics of acetylene decomposition

Eremin A V and Mikheyeva E Yu[@]

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

[@] ekaterina.mikheyeva@gmail.com

Acetylene is a unique exothermic hydrocarbon capable of detonating without oxygen. Hydrogen and hydrocarbon additives have been proposed as inhibitors of acetylene decomposition [1]. However, it was shown in [2] that small methane additives accelerate and increase the soot formation during the pyrolysis of acetylene. The promotion effect is explained by the formation of an additional kinetic channel for the formation of the first aromatic ring (benzene and phenyl) due to the recombination of the methyl radical with the acetylene molecule and the subsequent recombination of propargyl radicals. In this work, we studied the effect of various hydrocarbon additives, dissociating with methyl radical formation, on acetylene decomposition. Methane, ethane, dimethyl ether and diacetyl were considered. The calculations were carried out using kinetic mechanisms [3, 4] in the 0-dimensional approximation under constant volume conditions. The simulation results have shown that the effect of the considered additives on acetylene decomposition strongly depends on temperature. Under conditions of low temperatures, 1000–1200 K, and atmospheric pressure, the addition of dimethyl ether and diacetyl leads to a significant promotion of acetylene decomposition, while the addition of methane slows down the process. At higher initial temperatures, 1700–2000 K, methane addition is the most effective promoter and ethane addition is the best inhibitor of acetylene decomposition and subsequent soot formation. The kinetic reasons for these effects are discussed. This study was funded by the Russian Science Foundation, project No. 19-79-10204.

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Detonation properties of explosive proppants based on slurry nitromethane + ammonium perchlorate mixtures

Komissarov P V[2,1,@], Basakina S S[2], Lavrov V V[3] and Sokolov G N[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, Kosygina Street 4, Moscow 119991, Russia
[3] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia

[@] dot-dot@inbox.ru

The paper represents results of investigation upon detonation properties of heterogeneous mixtures of ceramic proppants with slurry liquid explosives such as nitromethane + ammonium perchlorate compositions (LE). The mixtures discussed are promised to be used for far field fracture stimulation of oil bearing formation subjected to hydraulic fracturing. Experimental results on detonation velocities of LE-proppant mixtures in long tubes up to 25 diameters versus internal diameters are presented. Results of experimental comparison of detonability of LE studied with pure nitromethane in proppant matrix is also represented. The objective of the study was to assess detonability and detonation parameters of these mixtures at various initial conditions.

Experimental research of ignition and combustion processes for boron mixtures with potassium and ammonium perchlorates in a free volume

**Shpara A P[1], Yagodnikov D A[1], Papyrin P V[1,@],
Sukhov A V[1], Storozhenko P A[2] and Huseynov S L[1]**

[1] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5,
Moscow 105005, Russia
[2] State Research Institute for Chemistry and Technology of Organoelement
Compounds, Shosse Entuziastov 38, Moscow 111123, Russia

[@] papyrin_pv@bmstu.ru

In various industries, powdered oxidizing agents and powdered met-
als are used. The purpose of this work is experimentally study the
features and determine characteristics the ignition and combustion
of gas suspensions boron-containing fuel particles in an open volume.
In this investigation, to assess possible solutions to the objectives
arising from the goal, the experimental study of the characteristics
of ignition and combustion of mixtures powdered oxidizer (PO) and
fuel (PF) carried out. Potassium perchlorate (PP, average parti-
cle diameter $d_k \approx$ 60–70 μm), and ammonium perchlorate (AP)
of two modifications—large AP1 ($d_k = 225$ μm) and small AP2
($d_k = 70$ μm) were used as PO. The PF was a boron of two types—
a nanoboron with an active boron content of 98.9% (specific surface
area of 18 m^2/g, calculated average particle diameter 0.142 μm)
and micron boron (mass average particle diameter 10.88 μm). Also
PF from aluminum diboride AlB$_2$ (mass-average particle diameter
9.03 μm) were used. The geometric characteristics of the flame
spread in a gas suspension a two-component mixture powdered PP
and AP as well as in a powdered fuel based on nano and micron
boron particles, depending on their concentration and dispersion
were experimentally determined.

Enhancement of particle shadow velocimetry technique experimental data postprocessing algorithm

Loginova A A[1,2,@] **and Chelebyan O G**[1]

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

[@] loginova.aa@yandex.ru

This paper is devoted to the droplet size and velocity measurement PSV (particle shadow velocimetry) technique [1] study and application. High-magnification shadow Imaging is very suitable for visualizing particles, droplets and other structures. The technique is based on high resolution imaging with pulsed backlight illumination [2]. This technique is independent of the shape and material (either transparent or opaque) of the particles and allows to investigate a particle size of 7 μm. Particle size, velocity, concentration, shape and distribution, mass flux can be obtained using PSV technique.

The enhancement of PSV technique experimental data postprocessing algorithm have been carried out. Using minimum slope filter the depth of field correction have been accomplished and this led to percentage error decreasing (deriving D10—from 33% to 2.5%; deriving D32—from 16.5% to 0.8%).

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Visualization of flame front propagation in the visible and infrared range

Elyanov A E[@], Golub V V and Volodin V V

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

[@] elyanov14@physics.msu.ru

Experiments on the visualization of the flame propagation in a lean hydrogen–air mixture were conducted. The flame was visualized using an infrared camera and a high-speed camera with a shadow device IAB-451. The main spectral mode of water steam emission is 2.7 μm and the location of combustion products is registered by the infrared camera. Shadow visualization of a flame is based on the deviation of a plane parallel beam of visible light on variations in the refractive index of the medium. It reveals the heat front ahead the flame. We suppose that the reaction zone is located between the heat front which is revealed by the shadow technique and the front of combustion products detected by the infrared camera. In this work we report the results of the investigation of the flame front and its wrinkled structure. The reported study was funded by the Russian Foundation for Basic Research within project No. 20-31-70041.

Stability of combustion waves in a two-layer solid fuel system

Miroshnichenko T P[@] and Gubernov V V

Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

[@] taisia.miroshnichenko@gmail.com

This work is devoted to the study of combustion regimes in a solid fuel system consisting of a pair of thermally adjacent layers. It is assumed that the materials of which the layers consist, differ in their thermophysics characteristics. However, they are able to interact with each other through a single-stage exothermic gasless reaction. A one-dimensional thermo-diffusion system consists of heat equations and chemical kinetics equations for each of the layers. Depending on the set of parameters, various combustion modes realized. Waves can move synchronously side by side or overtake one another. The overall velocity of the combustion wave and its structure depend on the layer in which the leading wave is formed. The leading wave leads to the appearance of super-adiabatic temperatures in the lagging wave, which is a very important property from the point of view of possible applications for the organization of combustion synthesis. The influence of the instabilities arising in each of the subsystems on the adjacent layer is investigated. The limits of instability of the general two-layer system are determined. The work is supported by the Russian Foundation for Basic Research (project No. 18-38-00523).

Flames under the reducing gravity

Krikunova A I

Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

krikunovaai@gmail.com

Combustion is traditionally investigated under conditions of normal gravity, reduced and induced one or of gravity jitter [1], while flame instability is not taken into account for variables not harmoniously oscillating g. However for the application area such conditions are pretty common, for example during plane or spacecraft landing or axis step. So the combustion instabilities under the transition conditions, is influenced the engines efficiency. This work is devoted to the numerical and experimental analysis of the methane-air conical flame behaviour under conditions of gravity change from normal one to microgravity.

Numerical simulation was provided using FlowVision software package [2]. An experiments were carried out on the Bremen Drop tower [3]. The stoichiometric methane–air flames with flow Reynolds number 600, 800, 1000 and 2000 were studied. It was shown high amplitude flame front oscillations, periodic flashback and hot spots separation during the first second of the capsule release in Drop tower. The results report the coincidence of the oscillations logarithmic damping decrements for different flow Reynolds numbers.

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Inverted conical flame dynamics

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

[@] krikunovaai@gmail.com

The stabilization of combustion of pre-mixed fuels is of great practical importance in a wide range of technical systems based on the use of flame. Understanding, describing and controlling the dynamic processes in such systems and especially the response of their functioning to external influences is an urgent task. The work considered open rich methane–air flames stabilized together by the thin edge of the burner and a cylindrical stabilizing body [1, 2]. The main goal was to study and compare the dynamics of the conical and reverse conical flames with the same hydrodynamic flow regimes. Numerical modeling was carried out using the finite element method using the FlowVision software package. The flow was formed in the burner, which is a conical nozzle with an output diameter of 15 mm. The nozzle parameters made it possible to obtain a rectangular exit velocity profile. At a distance of 3 mm from the inlet, a thin cylindrical stabilizer with a diameter of 2 mm was installed perpendicular to the flow. A comparative analysis of the results of numerical simulation for a conical reverse flame with classical conical flames is carried out, the dynamics of the velocity field and flame front are studied. It is shown that processes similar to those in a conical flame occur in a reverse conical flame, and the flame front is deformed due to the movement of Kelvin–Helmholtz vortices along the front. The constancy of the frequency of oscillations of the reverse conical flame is explained by the fact that the outer part of the M front is located in the mixing layer, where constant values of the coefficient of excess fuel are realized due to mixing of the combustible mixture with the surrounding air. Accordingly, in flames under the study, similar conditions of vortex formation are formed, which initiate low-frequency oscillations.

[1] Krikunova A I 2019 *Phys. Fluids* **31** 123607
[2] Krikunova A 2019 *High Temp.* **57** 430–7

V-flame dynamics

Krikunova A I[@] and Glushneva A V

Moscow Institute of Physics and Technology, Institutskiy Pereulok 9,
Dolgoprudny, Moscow Region 141701, Russia

[@] krikunova@phystech.edu

The passive method of stabilization of a premixed conical flame can change the shape of the flame in the form of M and V. The V-shaped flame could be formed in a wide range of fuel equivalence ratio and flow rate [1], therefore it is more widely used. However, the V-shape is more stable than the conical one, it is necessary to study the V-shaped region of flame stability and hardening processes [2]. Flame front flickering, stretching and curvature are the most important characteristics that describe flame dynamics and stability. This specific experimental work is devoted to the study of methane–air flame. The flame flickering frequency for various fuel equivalence ratio were measured for the normal and reversed gravity conditions. The results were provided within the Russian Foundation for Basic Research grant (project No. 18-31-00462).

[1] Krikunova A I 2019 *High Temp.* **57** 430–7
[2] Krikunova A I 2019 *Phys. Fluids* **31** 123607

Reactionary zones excited-state programming by plasma-acoustic coupling mechanism for the next-generation small satellite solid propulsion systems

Lukin A N

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

lukin@wcrc.ru

Small satellites are changing the game for deep space missions because can work together in a fleet to take on more complex missions. Smart control by excited-state of the reactionary zones is one of the keys to access to the properties of the solid propellants reactionary zones. In particular, the self-organized wave patterns excitation occurs at excited-state of the reactionary zones. On the base of detailed analysis we suggest the new concept for the reactionary zones programming, based on universal laws of cymatics and Unified Template approach of the self-organized wave patterns excitation phenomenon. Use of the plasma-acoustic coupling mechanism is one of the advanced ways to access to the properties of the reactionary zones: the scale and localization of the induction and energy-releasing areas. Application of a suggested understanding of the cymatic phenomena in the reactionary zones is opening the new ways for inertial-free control by the structure and properties of the reactionary zones with minimum expenses of energy. Suggested concept for manipulating by self-organized wave patterns and micro- and nano-scale oscillatory networks in the reactionary zones with using of new generation of the electrically activated solid propellants is opening the door for completely new ways for producing extremely small thrust impulses for the extra-precise attitude control of the small satellites.

Using data on shield volcanoes on Venus, craters on Mars, and seas on the Moon to determine the flux density of galactic comets in the Orion–Cygnus jet stream

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 Street 18, Kazan, Tatarstan 420008, Russia

[@] azary@mail.ru

With the use of data upon shield volcanoes on Venus, as well as upon the distribution of craters on Mars and sea basins on the Moon, the flux density of galactic comets in the Orion–Cygnus branch was calculated. The comets flux density is 5×10^{-10} (year km^2)$^{-1}$. This value was used to estimate the number, energy and fallings frequency of galactic comets on terrestrial planets in the period from ≈ 5 to 1 million years ago. It has been shown, that the falls of such comets can explain the phenomena of "newest uplifts of Earth's crust" and "young volcanism" on Earth, the appearance of shield volcanoes on Venus, the asymmetric structure of Mars, as well as origin of large craters, mares and mascons on the Moon, Mars and Mercury. A hypothesis of formation on the Moon of the South Pole–Aitken basin by galactic comets is proposed.

3. Power Interaction with Matter

Compressed laser-induced microplasma as an effective tool for transparent materials processing

Veiko V P[@], Samokhvalov A A, Gornushkin I B, Kostyuk G K, Sergeev M M, Shkuratova V A, Zakoldaev R A, Gresko V R and Koval V V

ITMO University, Kronvergskiy 49, Saint-Petersburg 197101, Russia

[@] vadim.veiko@mail.ru

The basic and applied interest in laser-induced plasma (LIP) has not faded for many decades. LIP is, in fact, a converter of laser energy into other ranges of radiation, the form of matter and motion. This is confirmed by such LIP applications as generation of soft x-ray radiation, laser motion, nanoparticle synthesis, coating (deposition) of thin films, impact hardening of metals, etc. However, this report focuses on a new version of LIP, namely, plasma obtained by laser ablation of a highly absorbing target in contact with a transparent solid medium—the so-called compressed laser-induced microplasma (CLIMP). CLIMP is basically a focused group of excited particles (electrons, ions, atoms and molecules), and its temporal and spatial parameters are completely determined by the characteristics of the laser beam and the parameters of the target along with the transparent material. Transparent material limiting the expansion of LIP is controlled by CLIMP, which leads to its accurate and efficient processing. At the presentation, the dynamics of CLIMP and its main parameters will be discussed. Choosing the proper wavelength it is possible to process a surface of different materials. We will consider the example of diffraction grating fabrication on a Si surface by CO_2-laser beam ($\lambda = 10.6~\mu$m) with a SiO_2 target. We will consider the use of CLIMP for the manufacture of a number of optical elements on the surface of fused silica, such as a microlens grating, a diffraction phase grating, and a new type of random phase-polarizing plate made on the surface of birefringent materials. The reported studies is funded by grant No. 074-U01 of the Government of the Russian Federation for ITMO University.

Laser technologies: From physics of ablation to surface nanostructuring and to synthesis of colloids

Inogamov N A[1,2]**, Zhakhovsky V V**[2]**, Khokhlov V A**[1,@] **and Petrov Yu V**[1,3]

[1] Landau Institute for Theoretical Physics of the Russian Academy of Sciences, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia
[2] Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya 22, Moscow 127055, Russia
[3] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] nailinogamov@gmail.com

Laser technologies cover a broad range of present-day industrial applications, from the automotive industry, shipbuilding and mechanical engineering to the printing of meta-surfaces for microelectronics, plasmonics, sensors, etc. In many cases these applications run ahead a physical theory which should support planning and optimization of production. Authors report here recently obtained results. They reveal hierarchies of physical processes taking place during synthesis of colloidal solutions of nanoparticles via ablation of metals in liquid and nanostructuring of metasurfaces. Evolution from early to late stages of ablation in liquid is followed. Influence of duration of a pulse is described. Dissolution–evaporation of metal atoms through a surface barrier into liquid and removal of this barrier at higher temperatures above critical temperature (surface tension decreases to zero) and transfer from dissolution and diffusion to pure diffusion are considered. Condensation of dissolved metal atoms inside dense environment (thus outside existing theories of nucleation) is studied.

Laser ablation of a multilayer target with layers of nanometer thickness

Khokhlov V A[1,@]**, Ashitkov S I**[2]**, Inogamov N A**[1,3,2]**, Komarov P S**[2]**, Parshikov A N**[3,2]**, Petrov Yu V**[1,4]**, Romashevskii S A**[2]**, Struleva E V**[2] **and Zhakhovsky V V**[3,2]

[1] Landau Institute for Theoretical Physics of the Russian Academy of Sciences, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[3] Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya 22, Moscow 127055, Russia
[4] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] v_a_kh@mail.ru

Multilayer products from ultrathin layers are widely used in modern science and technology. Laser irradiation is used as one of the promising methods for processing such products. In this paper, we study the ablation of a multilayer target of alternating layers of nickel and aluminum. A physical model is constructed, numerical simulation is performed, and experiments are carried out. The experiences are unique. Firstly, the reflection coefficient is measured. Secondly, the experiments were conducted in parallel with two different lasers with different diameters of the focusing spot. The first (when the laser radiation intensity increases from zero) breakdown occurs in the thickness of the first nickel layer, the second near the boundary of this layer and the first layer of aluminum. The threshold and depth of the first break obtained as a result of numerical (hydrodynamic) modeling correspond to experimental results with an accuracy of about 10%. This allowed us to refine the model of two-temperature states and determine the strength of nickel. It is explained why, with an increase in the absorbed fluence, first the upper layer breaks in the multilayer.

Nickel and aluminum as materials for the multilayer ablation: Electron thermal conductivity in solid and liquid phases in two-temperature states

Petrov Yu V[1,2]**, Inogamov N A**[1,3,@]**, Khokhlov V A**[1] **and Migdal K P**[3]

[1] Landau Institute for Theoretical Physics of the Russian Academy of Sciences, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[3] Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya 22, Moscow 127055, Russia

[@] nailinogamov@gmail.com

We investigate the ablation of multilayer targets under the influence of ultrashort laser pulses. The structure of strictly alternating layers of nickel and aluminum was taken as such a target. A short pulse duration leads to the appearance of a two-temperature states in metals with differing temperatures of electrons and ions and to the need to know the kinetic coefficients in this state for numerical simulation of ablation. Analytical expressions for the electronic thermal conductivity of nickel and aluminum are presented. The thermal conductivity coefficient depends on the electronic and ionic temperatures, density and phase of the substance (solid or liquid). The expressions obtained can be used in hydrodynamic calculations of the ablation of these metals or multilayer targets from them under the influence of ultrashort laser pulses.

Determination of 100 TW femtosecond laser contrast from measurements of specular reflectivity from solid target

Safronov K V[@], Flegentov V A, Gorokhov S A, Gavrilov D S, Kovaleva S F, Tischenko A S, Zamuraev D O, Shamraev A L, Mokicheva E S and Potapov 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

[@] konstantin.safronov@gmail.com

Temporal contrast is a crucial parameter for high-power short-pulse laser facilities. It influences on laser-driven ion acceleration [1], K_α radiation source properties [2], higher order harmonics generation [3]. Precise determination of the contrast is a challenging task. It requires measurements with dynamic range higher than 10^{10} in time interval of 10 ns with resolution of the order of the main pulse duration. A simple method for estimation of amplified spontaneous emission (ASE) prepulse energy was proposed in [4]. It is based on measuring brightness of specularly reflected from a solid target laser radiation on a scattering screen. Using this method, we investigated ASE contrast of 100 TW femtosecond laser facility before and after insertion of RG-850 saturable absorber into amplification chain. ASE intensity was also measured over delay times from -400 to 0 ps by a third order cross-correlator. Analysis of the images from scattering screen has shown that, in addition to ASE prepulse, contrast is affected by change of laser light absorption mechanisms at 10^{16}–10^{17} W/cm^2. This factor limits applicability of the method [4].

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Raman spectroscopy insight into surface modes of silicon nanoparticles

Povarnitsyn M E[1,@] and Shcheblanov N S[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Laboratoire Navier, Université Paris-Est, Ecole des Ponts-ParisTech, IFSTTAR, CNRS (UMR 8205), Allée Kepler 2, Champs-sur-Marne, Marne-la-Vallée F-77420, France

[@] povar@ihed.ras.ru

With the use of classical molecular dynamics, we model and study the vibrational properties of silicon nanoparticles, both crystalline and amorphous. With the help of Raman spectroscopy we reveal several important vibrational features. In particular, we find out low-frequency Raman lines related to the surface Lamb modes, and reveal that their locations correlate with the nanoparticle diameter. Moreover, vibrational spectra show that only the near-surface atoms contribute to the low-frequency Raman spectra. While, the high-frequency range is mainly formed by the core atoms and contains information about the phase state of nanoparticles. The obtained results can be used to analyse the size of nanoparticles.

The formation of nanomaterials by thermoplasmonics laser-induced backside wet etching

Zhigalina O M[1,2]**, Khmelenin D N**[1]**, Atanova A V**[1]**, Sviridov A P**[1] **and Tsvetkov M Yu**[1,@]

[1] Federal Scientific Research Centre "Crystallography and Photonics" of the Russian Academy of Sciences, Leninsky Avenue 59, Moscow 119333, Russia
[2] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

[@] mtsvet52@mail.ru

Currently laser ablation is the promising method for producing of various types of nanoparticles, and appropriate experiments are performed in a variety of configurations.

One of them is processing and structuring of transparent materials by focusing of the powerful laser radiation on the back surface of materials which contacting with a highly absorbing liquid media. Such technique is known as laser-induced backside wet etching (LIBWE). We developed this method using a solution of silver nitrate as an absorbing medium. Under the laser radiation a "cloud" of highly absorbing thermoplasmonics silver nanoparticles forms at the interface of the sample and $AgNO_3$ water solution.

This allows us to process a very hard material such as sapphire, nanostructuring and modification of its surface layer and to form various nanoparticles and clusters. The report presents results of a study of the structure and phase composition of the created plasmon nanostructures. Transformations of matter that occur in this case are discussed.

Ultrafast destruction of condensed and hollow optical fibers under laser action

Efremov V P

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

dr.efremov@gmail.com

Silica is optic material transmitting powerful laser fluxes. Damage of the light conductivity in the silica optical fiber transporting intense laser radiation leads to the absorption of energy and the appearance of a bright laser plasma with solid density. The plasma begins to move towards the radiation source, irreversibly damaging the light guide. Depending on driving laser energy, different damage propagation velocities are possible [1–5]. New scientific challenge is creation of extremal states inside hollow optical fibers under laser action [6].

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Landau levels of vacancions in two-dimensional Wigner crystal

Bisti V E

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

bisti@issp.ac.ru

The many-body problem for two-dimensional (2D) electron system (2DES) has no unified theoretical descriptions in the intermediate range of interaction parameter r_s neither for the ground state no for the elementary excitations. The ground state can be considered to be an electron gas, electron Fermi-liquid ore Wigner crystal. The liquid-solid transition calculations including the effect of impurities [1] give the possibility to consider 2DES as a Wigner crystal for $r_s = 6$–7. In the recent work [2] the photoluminescence spectra from the two-dimensional electrons (2DES) confined at MgZnO/ZnO heterojunction at $r_s = 6$ are studied. Electrons recombinate with the localized valence-band holes, and a quasiholes appear in 2DES. In the magnetic field there are well defined lines from Landau levels. But the unusual photoluminescence (PL) spectra transformation in the magnetic field for the lower-density samples is observed. The PL Landau-level fan looks "inverted". As it is shown in [3] it is possible to consider the quasiholes as vacancions in 2D Wigner crystal. In this work the energies of a vacancions in a magnetic field (Landau levels for vacancions) are considered in the quasiclassical approximation. It is shown that Landau levels from maximum and minimum sides of the bandgap depend differently on magnetic field. The energy level inside the band corresponding to the singularity point for the density of states does not depend on magnetic field. The picture for Landau levels is inverted if the 2D Wigner crystal has changed from the ferromagnetic to the antiferromagnetic state.

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Ab initio calculations of the electron-phonon coupling factor for crystals under nonequilibrium heating

Smirnov N A

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

deldavis@mail.ru

In this report, the results of calculations of the *ab initio* electron–phonon coupling coefficient for some metals (Cu, W, Pt, Au), whose electronic and ionic subsystems are heated under nonequilibrium conditions are presented. Instead of the formula by Wang *et al* [1994 *Phys. Rev. B* **50** 8016], which is often used to determine the temperature dependence of the electron–phonon coupling factor $G(T_e)$, we propose an inproved approach for its calculation from first principles. Comparisons with experiment and other calculations demonstrate good accuracy of our approach. In addition, the formula of Wang *et al* is shown to overestimate (up to a factor of 2) the extent of $G(T_e)$ variation at temperatures from 0.3 to 45 kK.

On role of electron–electron, electron–ion and electron–phonon interactions and interband transitions in optical properties of warm dens matter

Veysman M E[1,@], Röpke G[2,3] and Reinholz H[2,4]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] University of Rostock, Universitätsplatz 3, Rostock 18051, Germany
[3] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[4] University of Western Australia, Crawley WA6009, Australia

[@] bme@ihed.ras.ru

The method of quantum statistical operator and the linear response theory [1] is used for derivation of expressions for real and imaginary parts of correlation functions, dynamical conductivity and permittivity for warm dens metter with both ordered [2–4] and disordered [4,5] ion system. That gives one possibility to obtain simple models of kinetic coefficients which can be used for simulations of powerfull laser pulses interaction with matter for wide range of laser and created plasmas parameters and to studdy optical properties of laser heated matter. The influence of Umklapp process, electron-phonon interactions and intraband transitions on optical properties of metallic plasmas at different wavelength of laser radiation and different temperatures of ion and electron component of the plasma is discussed using created models.

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Kinetic simulation of the electron heat wave propagation induced by inverse bremsstrahlung heating in a laser-produced plasma

Karpov S A[1,@]**, Potapenko I F**[2] **and Bychenkov V Yu**[1,3]

[1] Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya 22, Moscow 127055, Russia
[2] Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, Miusskaya Square 4, Moscow 125047, Russia
[3] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

[@] karpov.st@yandex.ru

In a laser-heated plasma, features such as a steep temperature gradient, nonlocal heat transfer, and suprathermal electrons are common and are of constant interest for thermonuclear fusion (ICF). In this work we present the results of numerical kinetic simulation of the electron heat wave propagation induced by inverse bremsstrahlung heating in a laser-produced plasma. Simulations have been performed with the original finite difference numerical code which solves the nonlinear one-dimensional two-velocities Fokker–Planck kinetic equation with a self-consistent electric field [1,2]. The temperature, heat flux profiles and the non-equilibrium electron distribution function in the velocity space have been studied in details. The results of kinetic simulations significantly differ from that manifesting in hydro-simulations. We also make an estimate of the hot electrons contribution to the particle number density and mean energy, their influence on plasma preheating and plasma wave Landau damping that is important for ICF laser-plasma interactions.

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Generation of relativistic electrons and gammas in the interaction of relativistic laser pulses with plasma of near critical density

Andreev N E[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 141701, Russia

andreev@ras.ru

Experiments upon the efficient laser acceleration of electrons in long scale plasma of near critical density were carried out at the PHELIX laser facility at GSI, Darmstadt. Low density polymer foam layers of 300–450 μm thickness and combination of foams with μ-thin up to mm-thin plane metallic foils were used as targets. In foams, the near critical electron density (NCD) plasma was produced by a mechanism of super-sonic ionization when a well-defined separate ns-pulse was sent onto the foam-target forerunning the relativistic main pulse. The observed strong increase of the energy and the number of ultra-relativistic electrons is reinforced by the results of gamma-yield measurements that showed a 1000-fold increase of the measured doses. The experiment was supported by the 3D-PIC (three-dimensional particle-in-cell) and FLUKA simulations. Using a combination of the foam layers with mm thick high Z convertors at 10^{19} W/cm^2 laser intensity we detected gamma-driven nuclear reactions with a γ-energy threshold up to 23 MeV. Measured reaction yield was higher than in the case of the direct shots on to similar convertor foils at 10^{21} W/cm^2 laser intensity. These results open new perspectives for the laser driven particle acceleration and nuclear photonics already at relativistic-moderate laser intensities. This work was partially supported by the Presidium RAS within program "Extreme light fields and their interaction with matter" and the Russian Foundation for Basic Research (project No. 19-02-00908).

Nonlinear processes in the injection and acceleration of electrons in plasma wake field in the interaction of a subterawatt laser pulse with a gas jet

Popov V S[1,2,@] **and Andreev N E**[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 141701, Russia

[@] SlavaPopov1991@yandex.ru

The effect of nonlinear self-focusing and self-modulation processes upon the acceleration of electrons of a subterawatt femtosecond laser pulse with a gas jet plasma was considered. A three-dimensional particle-in-cell (3D PIC) simulation of the interaction of laser radiation with a low-density nonuniform plasma shows that at the moment when the laser pulse reaches the region with plasma concentration, where the laser pulse power approaches the critical power of relativistic self-focusing, the laser pulse is compressed, which leads to an effective generation of the plasma wave. Due to a decrease in the phase velocity of the wake plasma wave generated via self-modulation of the laser pulse, electrons are trapped into the accelerating phase of the plasma wave and are accelerated to energies of 10 MeV. It is shown that under the conditions for limiting the interaction region of the plasma wave with the injected electrons by the length of their dephasing, quasimonoenergetic electron bunches with a characteristic energy of 9 MeV can be produced. Thus, it is possible to obtain electron beams in the laser-plasma injector for their further effective acceleration. The effective temperature of the accelerated electrons and their angular distribution, obtained by 3D PIC simulation, are in good agreement with those determined in the experiment.

Generation of wake fields by femtosecond laser pulses in an inhomogeneous plasma of a gas jet

Umarov I R[1,2,@] **and Andreev N E**[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 141701, Russia

[@] umarov.ir@phystech.edu

The interaction of a short high-intensity laser pulse with an Ar gas jet is considered taking into account optical ionization. Modeling in three-dimensional cylindrically symmetric geometry was performed for various moderately relativistic intensities and positions of the focal plane of the laser pulse both in the case of optical gas ionization and in the case of pre-ionized plasma. The influence of the processes occurring during optical ionization of a gas on the generation of wake waves is studied, and the conditions are found under which the generation of intense wake fields in a plasma formed from an inhomogeneous argon gas jet occurs. The possibility of using a gas with a large number of electrons on the outer shell (argon in this case) to excite wake waves and accelerate electrons is demonstrated. Despite the significant ionization diffraction of the laser pulse by the radially inhomogeneous plasma density profile formed by optical ionization, the region of the parameters of the laser pulse and the gas target is determined for which ionization refraction leads to the generation of an intense wake wave when in a pre-ionized plasma for the same laser intensity generation of a wake wave does not occur.

Generation of electron bunches by an ultrarelativistic laser pulse intersecting the boundary of inhomogeneous plasma

Kuznetsov S V

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

shenau@rambler.ru

An important problem in the practical implementation of a laser-plasma accelerator providing monoenergetic acceleration of electron bunches is the generation of short electron bunches for acceleration. An interesting phenomenon in the generation of electron bunches of attosecond duration was discovered in [1] in the numerical simulation of the propagation of a high-power laser pulse in an inhomogeneous plasma. It was supposed that the laser pulse is incident normally on a diffuse plasma boundary comprising a transition layer in which the plasma density varies linearly with plateauing out. It turned out that, when the laser pulse amplitude exceeds a certain threshold value in the neighborhood of the point at which the plasma density reaches the plateau, a quasi-one-dimensional process of generation of electron bunches develops. For the case of a sharp plasma boundary, a theoretical analysis of this phenomenon in one-dimensional geometry is proposed in [2,3] on the basis of a simple physical model in which plasma electrons are considered as plasma oscillators whose one-dimensional motion is excited by a laser pulse. A generalization of the theory [2,3] for the case when the plasma boundary as in [1] has a linear transition layer is presented in [4].

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Experimental investigation of relativistic electron beam generation in glass capillaries under the action of ultra-intense laser pulse

Gorokhov S A[@], Flegentov V A, Safronov K V, Kakshin A G, Gavrilov D S, Loboda E A and Pkhaiko N A

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

[@] dep5@vniitf.ru

Laser plasma is able to produce very high acceleration wakefields, enabling compact accelerators generating high brightness ultra-shot particle beams. "Table top" laser could potentially deliver relativistic electron bunches for variety of application, including production of intense gamma ray burst for high density object radiography. The main problem to date is to increase the electron acceleration efficiency. This goal can be achieved by suitably tailoring acceleration plasma structure to allow of guiding a high laser pulse. Inside capillary, it is possible to create an axisymmetric plasm density distribution to assist guiding [1]. We report the result of experiments on electron acceleration from capillary targets which were performed on 30 TW picosecond laser facility. Accelerating plasma medium was created by ablating capillary inner walls with specially generated prepulse at 1.2 ns before the main pulse. We measured electron bunch spectra and divergence at different capillary diameters and prepulse energy. It was found that for every capillary diameter the exists an optimal prepulse when accelerated particles are observed. We detected relativistic electron beams of exponential spectrum with energies of up to 20 MeV, 50 mrad divergence angle and total charge of 200 pC.

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X-ray time-resolved diagnostics of hot electrons generation in shock ignition relevant experiments

Martynenko A S[1,2]**, Filippov E D**[1,3]**, Renner O**[4,5]**, Antonelli L**[6]**, Baffigi F**[7]**, Chodukowski T**[8]**, Cristoforetti G**[7]**, Dudzak R**[4,5]**, Gizzi L A**[7]**, Juha L**[4,5]**, Krupka M**[5]**, Krus M**[4,5]**, Mancelli D**[9]**, Ospina V**[9]**, Pikuz S A**[1,2,@]**, Pisarczyk T**[8]**, Rusiniak Z**[8] **and Batani D**[2,9]

[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 of Applied Physics of the Russian Academy of Sciences, Ulyanova 46, Nizhny Novgorod 603950, Russia

[4] ELI Beamlines, Institute of Physics of the Czech Academy of Sciences, Za Radnicí 835, Dolní Břežany 25241, Czech Republic

[5] Institute of Plasma Physics of the Czech Academy of Sciences, Za Slovankou 3, Prague 18200, Czech Republic

[6] York Plasma Institute, Department of Physics, University of York, Church Lane, Heslington, York YO10 5DQ, United Kingdom (Great Britain)

[7] National Institute of Optics of the National Research Council, Largo Enrico Fermi 6, Firenze 50125, Italy

[8] Institute of Plasma Physics and Laser Microfusion, Hery Street 23, Warsaw 01-497, Poland

[9] Center for Intense Lasers and Applications, University Bordeaux, Cours de la Libération 351, Talence, Bordeaux 33405, France

@ spikuz@gmail.com

Detailed mechanisms for generating hot electrons are of great interest in connection with its importance for the formation of strong shocks and the approach to ignition of shocks for thermonuclear fusion. We used an x-ray streak-camera and spherically bent diffraction crystals to obtain time-resolved data of K-shell emission of the solid matter heated by a flow of hot electrons generated by a laser of shock-ignition relevant intensity of about 1.5×10^{16} W/cm^2 at the PALS facility. The analysis of this time-resolved emission dependencies on the laser parameters is presented.

The clean source of soft x-ray radiation generation in supersonic Ar gas jets by high-contrast femtosecond laser pulses of relativistic intensity

Alkhimova M A[1,@]**, Ryazantsev S N**[1,2]**, Skobelev I Yu**[1,2]**, Boldarev A S**[3]**, Feng J**[4]**, Xin L**[4]**, Li-Ming Ch**[4] **and Pikuz S A**[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] Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, Miusskaya Square 4, Moscow 125047, Russia
[4] Institute of Physics of the Chinese Academy of Sciences, Beijing 100190, China

[@] maalkhimova@mephi.ru

Laser-produced plasma as a bright, point-like, pulse source of x-ray radiation at the energy range of 0.1 to 50 keV is actively investigated last decades. In this work we optimized a clean, versatile, compact source of soft x-ray radiation ($E_{\text{x-ray}} \approx 3$ keV) with an yield per shot up to 7×10^{11} photon/shot in a plasma generated by interaction of high-contrast femtosecond laser pulses of relativistic intensity ($I_{\text{las}} \sim 10^{18}$–$10^{19}$ W/cm^2) with supersonic argon gas jets. Using high-resolution x-ray spectroscopy approaches, the dependence of main characteristics and the emission efficiency of the x-ray source on laser pulse parameters and properties of the gas medium were studied. The optimal conditions, when an x-ray photon yield reached maximum, have been found when the argon plasma has an electron temperature of $T_e \approx 220$ eV, an electron density of $N_e \approx 6 \times 10^{19}$ cm^{-3}. In such a plasma, a coefficient of conversion to soft x-ray radiation with energies $E_{\text{x-ray}} \approx 3.1 \pm 0.2$ keV reached 8.57×10^{-5}, and no processes leading to the acceleration of electrons to MeV energies occurred.

Characterization of high spatial resolution lithium fluoride x-ray detectors

Makarov S S[1,2,@]**, Pikuz T A**[1,4]**, Pikuz S A**[1,6]**, Mabey P**[3]**, Albertazzi B**[3]**, Michel Th**[3]**, Rigon G**[3]**, Ozaki N**[5]**, Matsuoka T**[5] **and Koenig M**[3,5]

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

[2] Department of Physics, Lomonosov Moscow State University, Leninskiye Gory 1 Bldg 2, Moscow 119991, Russia

[3] Laboratoire pour l'Utilisation des Lasers Intenses, CNRS-CEA, École Polytechnique, Physique Atomique dans les Plasmas Denses, Route de Saclay, Palaiseau F-91128, France

[4] Open and Transdisciplinary Research Initiative, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

[5] Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

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

[@] seomakarov28@gmail.com

The response of LiF crystal detectors to monochromatic x-rays is measured in the range of several kiloelectron-volts. This response, as a function of the x-ray dose, is independent of photon energy with no saturation level found. The response, as a function of the incident energy flux, is found to increase for photons of lower energy due to the differing attenuation lengths of x-ray photons within the crystal. Small differences are seen between different confocal microscopes used to scan the data, suggesting the need for absolute calibration. The spatial resolution of the LiF is also measured (1.19–1.36 μm) and is found to be independent of incident photon energy. Finally, a photometric study is performed in order to assess the feasibility of using these detectors at current x-ray free electron laser and laser facilities worldwide.

High-precision spectroscopy of x-rays emitted by laser plasma of heavy multiply charged ions

Ryazantsev S N[1,2,@]**, Skobelev I Yu**[1,2]**, Mishchenko M D**[1,2] **and Pikuz S A**[1,2]

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

[@] sergryaz@mail.ru

It is very important to know the exact wavelengths of radiative transitions in multiply charged ions in order to ensure effective x-ray spectroscopy for plasma diagnostics. It requires exact knowledge about a dispersion curve of a spectrometer applied for the measurements. The curve can be obtained by observing of investigated lines and lines with well-known wavelengths (references) in the same range simultaneously. For the case of focusing spectrometer with spatial resolution [1] the dispersion curve can be precisely fitted with a parabola. Thus, three reference lines are required for observations. H-like ions spectral lines are the best candidates for using as references, because it is always possible to calculate its wavelength with accuracy higher than the best experimentally available. But H-like ions lines appear for a rather narrow plasma temperature range and sometimes it is hard to observe them simultaneously with, for example, He-like ions lines of the same element. We propose to irradiate by laser pulses targets with a complicated chemical composition to avoid the problem. Exact experimental schemes are discussed for the purposes of measuring the He-like K XVIII ions radiative spectrum on the base of reference lines emitted by Al XIII and Si XIV H-like ions.

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Is quantum field theory complete?

Saikhanov M B

Ibragimov Complex Institute of the Russian Academy of Sciences,
Staropromyslovsky Avenue 21a, Grozny, Chechen Republic 364051, Russia

saikhanov_musa@mail.ru

The remarkable achievements of quantum field theory in studies of the fundamental structure of matter are now well known and are not in doubt [1]. This theory is based on the same principles and formalism of quantum mechanics that were originally formulated in the study of the structure of an atom. It turned out that under certain assumptions, which subsequently received experimental confirmation, they can also be successfully applied at the subatomic level for the theoretical description of electromagnetic, nuclear, and weak interactions, as well as the emergence, annihilation, and mutual transformation of elementary particles [2,3]. However, since the quantum field theory was created on the basis of quantum mechanics and therefore inherited one significant drawback from it, namely: it is not suitable for describing some of its objects in which nonequilibrium irreversible processes play a significant role. The latter include, for example, the processes of mutual transformation of elementary particles. Therefore, in this work, an attempt is made to expand the quantum field theory based on the modern theory of nonequilibrium irreversible processes, including away from equilibrium, which was significantly developed thanks to Prigogine, Nicolis and many other researchers [4–6].

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Correspondence between classical and quantum description of the radiation damping of ultra-relativistic electrons in oriented crystals

Khokonov M Kh

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

khokon6@mail.ru

As is well known, the classical radiation damping formula consists of two terms, usually called the terms "the Schott" and "Liénard". The Schott term is included in the expression for radiation self-force in the form of the total time derivative of the quantities that determine the motion of the particle [1]. This means that it cannot be directly measured in experiments. Nevertheless, the recent reports on the feasibility of detecting experimentally the effects of the action of classical radiative self-force on the motion of electrons (positrons) channelled in oriented crystals at the CERN Secondary Beam Areas (SBA) beamlines, indicate that the Schott term can be measured directly [2].

We give for the first time the quantum interpretation of classical radiation reaction coming from the near electromagnetic self-force (i.e., from the "Schott term") [3]. We show that quantum transitions between the transverse energy states of ultra-relativistic electrons channelled in oriented crystals represent the quantum analog of the classical Schott term, whereas the Liénard term is responsible for the total radiation energy losses. This type of radiation is unique in that sense that it has a pronounced quantum character in two extreme cases of low and high energies.

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Restoring size of detonation nanodiamonds from small angle x-ray scattering of polychromatic syncrotron-radiation beam

Rubtsov I A[1,@], Ten K A[1], Pruuel E R[1], Kashkarov A O[1], Zubavichus Y V[2], Peters G S[3] and Veligzhanin A A[3]

[1] Lavrentyev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 15, Novosibirsk 630090, Russia
[2] Boreskov Institute of Catalysis of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 5, Novosibirsk 630090, Russia
[3] National Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia

[@] rubtsov@hydro.nsc.ru

Time-resolved small angle x-ray scattering (TR-SAXS) experiments on detonating high explosives have being jointly conducted by the LIH SB RAS and BINP (Budker Institute of Nuclear Physics) SB RAS during last two decades. The purpose of these experiments is to restore the dynamics of carbon species condensation to diamond nanoparticles by analyzing series of SAXS patterns behind the detonation front measured in real time with fast detectors. This knowledge is crucial for the development of reliable detonation models. In this paper, we report comparison of SAXS patterns of identical nanodiamond samples measured at the TR-SAXS extreme state of matter end-station (BINP SB RAS) in the static mode under realistic conditions simulating fast real-time measurements with polychromatic syncrotron-radiation (SR) beam and traditional SAXS BioMUR beamline at the Kurchatov Synchrotron Radiation Source (NRC "Kurchatov Institute") with monochromatic SR beam. These experiments confirm that the size of scattering inhomogeneities determined in dynamic experiments with single bunch exposure with polychromatic SR beam is correct.

Radiographic complex in the Russian Federal Nuclear Center—VNIITF

Petrov D V[@], Garmashev A Yu, Smirnov E B, Nikitin O A and Kolesnikov P A

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

[@] snzjones@mail.ru

RFNC-VNIITF has developed a radiographic complex for studying high-intensity processes. The complex includes radiographic facilities with "soft" and "hard" spectrum bremsstrahlung radiation. Radiographic complex is intended for joint diagnostics of high-intensity processes and extreme states of matter using state-of-the-art techniques based on various physical principles.

This paper compares RFNC-VNIITF radiographic facilities to the ones used in top research laboratories in the world. The paper also considers the potential of RFNC-VNIITF radiographic complex and the results of the experiments conducted witch its help.

Cell proliferation under intense pulses of terahertz radiation

Sitnikov D S[1,@], Ilina I V[1], Revkova V A[2], Konoplyannikov M A[2], Kalsin V A[2] and Baklaushev V P[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Federal Research and Clinical Center of Specialized Medical Care and Medical Technologies of the Federal Medical and Biological Agency of Russia, Orekhovy Boulevard 28, Moscow 115682, Russia

[@] sitnik.ds@gmail.com

The use of terahertz (THz) radiation is growing rapidly both in basic research and in various practical fields (security and military use, medicine, etc). Nevertheless, concerns have been expressed about the possible health impacts associated with THz radiation. The use of high-power THz sources in biological studies may lead to major advances in understanding biological systems and help to resolve controversies over mechanisms of biological organization.

High peak power is required in order to overcome the strong THz absorption of water, penetrate the culture medium, and reach the cells. At the same time the average power needs to be low to avoid thermal effects, which could mask other intracellular changes. Here we present an experimental setup for long-term irradiation of cells with high-power THz pulses with intensities of about 32 GW/cm^2 [1] providing average power value as low as 1.5 mW.

Human skin fibroblasts were exposed to powerful THz pulses with a field strength of about 3.5 MV/cm for 90 min and divided into two experimental subgroups differed in fixation time after the irradiation—0.5 and 24 h. It has been demonstrated that the effect of THz radiation on cultured fibroblasts consists in the activation of the cascade of proapoptotic enzymes and inhibition of the ROS action on cells, not leading to cell apoptosis.

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Impact of strong picosecond THz pulses on p-silicon

Mishina E D[1,@], Kudryavtsev A V[1], Agranat M B[2], Ovchinnikov A V[2] and Chefonov O V[2]

[1] MIREA—Russian Technological University, Vernadskogo Avenue 78, Moscow 119454, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] mishina_elena57@mail.ru

In semiconductors, high electric fields produces electrical breakdown due to avalanche of electrons generated by impact ionization. This effect has been studied for decades in electronic devices in CW or low frequency field. Picosecond THz pulse with peak electric field strength which ranges up to tens of MV/cm gives birth to absolutely new effects, when impact ionization takes place but does not lead to breakdown because of high localization in time and space. In this paper, we utilize optical pump probe scheme in which THz pulse is used as a pump, and a femtosecond optical pulse is used as a probe. For detection, the second harmonic (SH) of the optical pulse generated in a p-type silicon crystal is used as a measure of THz pulse induced effects. For explanation, several possible effects are discussed and compared: (i) electric-field induced SH, (ii) nonlinear susceptibility changes due to transient carrier density increase and (iii) transient electric current induced SH; two latter effects arising due to impact ionization.

Laser generation of strong field THz and x-ray pulses for pump-probe experiments

Nazarov M M[1,@], Sheglov P A[1], Garmatina A A[1] and Margushev Z Ch[2]

[1] National Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia
[2] Kabardino-Balkar Scientific Center of the Russian Academy of Sciences, Inessa Armand 37, Nalchik, Kabardino-Balkaria 360051, Russia

[@] nazarovmax@mail.ru

Progress in laser physics allows to obtain ultra-short electromagnetic pulses with MV/cm quasi-static electric field, that is a conversion of tens of mJ femtosecond (fs) laser pulse into μJ THz one. Such pulses are capable to induce a unique non-stationary state of the matter without destroying it. To probe atomic lattice rearrangement on a fs-time scale x-ray diffraction can be used. Obtaining bright fs x-ray pulses synchronized with laser ones is a big challenge. We use TW laser pulses propagating as a filament to generate x-rays by metal target ablation [1] and the same pulses to generate THz in two-color induced gas plasma [2], all in a low-pressure gas chamber. Another big challenge is to refocus highly divergent x-rays from the target to the sample. For this purpose, we designed and manufactured a poly-capillary x-ray lens [3]. Experimental results on strong-field THz generation in a gas plasma, on x-ray generation in a copper foil, on a poly-capillary x-ray lens tests will be analyzed.

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Landau–Khalatnikov equation in case of strong picosecond THz pulse

Sherstyuk N E[@], Bilyk V R, Grishunin K A and Mishina E D

MIREA—Russian Technological University, Vernadskogo Avenue 78, Moscow 119454, Russia

[@] nesherstuk@mail.ru

One of the most important properties of ferroelectrics is their strong interaction with electromagnetic radiation, which is expressed in a number of photo-induced effects associated with ferroelectric polarization. In this connection effect of strong terahertz pulses on a charge subsystem of ferroelectrics which can lead to polarization switching (or modulation) is of most interest for the practical use. The dynamic response in nonlinear media under the influence of electromagnetic pulses can be examined using the Duffing equation (the anharmonic oscillator equation). Formally, the Duffing equation can be reduced to the Landau–Khalatnikov equation by renormalizing the coefficients.

In this report, a theoretical study of polarization dynamics under the influence of THz pulses on a $Ba_{0.8}Sr_{0.2}TiO_3$ is considered. Numerical solutions of the Landau–Khalatnikov equation using constants of thermodynamic potential for this material are show that the action of intense THz pulses leads to polarization modulations and strong nonlinear response. Dynamic polarization switching occurs under the action threshold value of about 400 kV/cm and agrees well with previous experimental results [1].

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Modeling of the second optical harmonic dynamics in silicon under the simultaneous influence of infrared femtosecond laser pulses and strong THz radiation

Kudryavtsev A V[@], Morozov V G and Mishina E D

MIREA—Russian Technological University, Vernadskogo Avenue 78, Moscow 119454, Russia

[@] oldousavk@yandex.ru

The results of modeling the dynamics of second harmonic generation (SHG) in silicon under the simultaneous action of infrared femtosecond laser pulses and powerful terahertz radiation with a field strength of up to 12 MV/cm are presented. Our model is based on the Boltzmann equation with taking into account the impact ionization process, the band structure of silicon, the THz impulse waveform, and the charge carriers relaxation and recombination times in silicon under considering conditions. It is shown that the features of the SHG dynamics are explained by impact ionization dynamics in the electric field of THz pulse. The developed model is in good agreement with the experimental results obtained in THz pump–optical (SHG) probe geometry in p-doped silicon, when THz pulses with a peak electric field strength in the range from 1.8 to 12.5 MV/cm used as the pump, and the SHG signal produced by femtosecond laser radiation at a wavelength of 1240 nm used as a probe.

Microwave action on the synthesis of nanocomposites selenium–polymer–surfactant

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

[@] svs@igm.nsc.ru

Nanosized selenium has a lot of wonderful properties connected with semiconductor and antioxidative abilities independent of modification. As for amorphous selenium it has the large scope of application in medicine, pharmacology as progressive drugs component, and in electronics as amorphous semiconductor. Red amorphous nanoselenium is especially attractive as biologically active component. In spite of toxicity it can be successfully used in therapy of cancer, arthritis, brain and heart illnesses, endocrine problems. Microwave action is interesting new tool for acceleration of chemical reactions. We used this action for synthesis of polymeric composites, containing nanoselenium. In the microwave reactor glass vessel with mixture of water solutions of polymer, selenium compound, reducing agent and ionogenic surfactant was placed. Different salt additives were tested also. After microwave treatment produced solutions were studied with methods of optical and electronic microscopy, uv-viz and Raman spectroscopy. Selenium stabilization can be explained with point of view conception of double electrical layer, since the latter property is a fundamental feature of an ionic surfactant.

Parameters determination of the sodium chloride radiative destruction area by femtosecond laser pulses

Savintsev A P[@] and Gavasheli Yu O

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

[@] savinal@mail.ru

In this work, the action of laser pulses (thermomechanical ablation) with a duration 80 fs at a wavelength of 1240 nm on crystals of sodium chloride was studied [1, 2]. The experiments were carried out at the Center for Collective Use of Unique Scientific Equipment "Laser Femtosecond Complex" at the Joint Institute for High Temperatures RAS, on the terawatt fs chromium–forsterit laser system [3]. Using an image processing program, the geometric dimensions R_x and R_y (lengths of the principal axes) of the damage spots were determined; they took the form of an ellipse due to the oblique incidence of the radiation on the target. It has been discovered that a linear dependence of the optical damage spot area (S) in the laser pulse energy (G) is higher than the crystal damage threshold: $S = K \ln(G/G_0)$, where G_0 is the energy of the optical damage and $K = \text{const}$. For sodium chloride, $G_0 = 105\ \mu\text{J}$, and $K = 1800\ \mu\text{m}^2$.

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First tests of laser ignition in Wankel engine

Loktionov E Y[@] and Pasechnikov N A

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

[@] yagor@bmstu.ru

Laser ignition was studied in powerful four-stroke engines, not only because of the quick payback, but also because of more convenient diagnostics in a large-scale installation. High-performance compact engines were not studied, albeit advantages of laser ignition could be even more pronounced for those because of harmful emission reduction and multi-fuel abilities.

Compact piston engines are seen as an alternative for fuel cells and batteries for portable, automotive and unmanned aerial vehicles. Those are characterized by small combustion chamber comparable to spark plug inter-electrode gap in axial direction, and its low ratio to bore size. For Wankel engines this problem exists at any scale though. Laser ignition of lean fuel mixtures in such engines could significantly improve performance by reduced fuel consumption, thermal loads, and cleaner exhaust.

We have investigated possibility of laser ignition in rotary-piston (Wankel) 1 hp scale model engine using different kinds of fuel mixtures: hydrogen, methane, propane, butane, gasoline, and ethanol based. A custom built compact end-pumped diode-pumped solid-state 2.7 mJ laser has been used to substitute original glow plug, respectively. Laser ignition has been found possible and quite beneficial for both types of engines and different fuel mixtures. In terms of NO_x emission reduction especially.

Active Brownian motion of emulsion droplets when exposed to laser radiation

Svetlov A S[1,2,@]**, Kononov E A**[1,2]**, Vasiliev M M**[1,2] **and Petrov O F**[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 141701, Russia

[@] svetlov.anton.s@gmail.com

The results of an experimental study of the nature of the motion of polydisperse droplets of an emulsion containing carbon submicron particles when exposed to laser are presented.

To study the nature of the motion in the obtained emulsion systems, the emulsion droplets were exposed to laser radiation, their motion was observed using a stereo microscope and recorded by a video camera. As a result of processing the experimental video data, the coordinates of the emulsion droplets for each moment of time were obtained, the distribution of the emulsion droplets in terms of speed along and across the video frame was obtained, and the mean square displacement and linear displacement along and across the direction of movement of the emulsion droplets were measured.

In experiments, the movement of polydispersed droplets of emulsions containing carbon particles was observed when exposed to laser radiation. Carbon particles can effectively absorb laser radiation, as a result of which the resulting photophoretic force can cause the movement of these particles inside the emulsion droplet, which leads to the movement of the emulsion droplets themselves.

It has been experimentally established that when the laser radiation acts on the droplets of the emulsion, the linear displacement along the direction of motion is larger than average droplet size, while the linear displacement across the direction of motion within an error equal to 0. Thus, we can conclude, that the motion of emulsion droplets containing submicron carbon particles is active Brownian.

Laser ablation on the coatings of hafnium and zirconium dioxides

Mkrtychev O V[1,@], Shemanin V G[1] and Shevtzov Yu V[2]

[1] Novorossiysk Branch of the Shukhov Belgorod State Technological University, Mysknakskoye Shosse 75, Novorossiysk, Krasnodar Region 353919, Russia
[2] Nikolaev Institute of Inorganic Chemistry of the Siberian Branch of the Russian Academy of Sciences, Academician Lavrentyev Avenue 3, Novosibirsk 630090, Russia

[@] oleg214@ya.ru

The authors previously conducted studies of various aspects of laser ablation related to the probabilistic nature of ablative destruction of nanoscale coatings on glass samples [1–4]. Statistical regularities of breakdown on absorbing defects were considered in the Weibull–Gnedenko model. In this paper, the authors investigated the dynamics of laser ablative destruction of hafnium and zirconium dioxide coatings on glass and silicon substrates. Threshold energy densities of laser ablation and various regularities connecting these threshold values with geometrical and optical parameters of irradiated materials were measured. Experimental studies of threshold energy densities of pulsed laser destruction of materials under the action of YAG-Nd laser radiation at wavelength of 1.064 μm and pulse duration of 20 ns were conducted. The results obtained make it possible to predict the behavior of such materials under the conditions of their irradiation with powerful pulsed laser radiation.

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Creation of heterogeneous cermet structures from stainless steel and WC by cold spray and followed laser treatment

Fomin V M, Shikalov V S[@], Kosarev V F, Orishich A M, Golyshev A A, Malikov A G and Filippov A A

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

[@] v.shikalov@gmail.com

Combined method for creating a heterogeneous coating based on powders of stainless steel and tungsten carbide, which consists of the sequential use of cold spray and laser treatment, is investigated. The maximum WC content in cold sprayed composite coating was reached equal to 0.38 of weight (0.24 of volume). For the first time, the optimization of laser treatment of cold sprayed stainless steel + WC coating was carried out. The preliminary results of the formation of cermet structures and its microstructure depending upon the parameters of laser treatment (power density, beam traverse speed, thickness of the fused layer, etc) are presented. The results obtained open up prospects for creating cermet structures containig metal matrix and reinforcing ceramic admixture with aid of combined method consisting of cold spray and subsequent laser treatment.

Influence of preliminary heat treatment and ball milling of aluminum powder on cold spray process

Klinkov S V, Kosarev V F, Shikalov V S, Vidyuk T M[@], Chesnokov A E and Smirnov A V

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

[@] vidyuk@itam.nsc.ru

Cold spraying is a low-temperature deposition technology in which powders are accelerated by gas passing through a De Laval supersonic nozzle and act on the substrate at high speed. In cold spray, the feedstock remains solid state (without melting) during the coating build-up process due to relatively low temperature of the driving gas. Initially, commercially available metal powders were used for cold spraying. This paper presents the results of a study of the effect of preliminary high-energy effects, such as: heat treatment and ball milling of aluminum particles on the cold spraying process (in particular, on the deposition coefficient), the structure of the sprayed coatings, and their physical properties. It is shown that the ball milling of aluminum powder in a planetary mill leads to a change in particle size and shape. Agglomerated particles with a layered structure are formed with closed microcracks and micropores in their volume. It was found that ball milling of the powder leads to an increase in the specific surface, a decrease in apparent density, and a decrease in the values of the crystallite size. X-ray diffraction patterns of the initial, heat treated and ball milled powders did not reveal a change in the phase composition. Profilometry of cold sprayed coatings did not reveal significant changes in the shape of coatings and their characteristic sizes (width, thickness), which indicates the absence of significant changes in the deposition coefficient of aluminum powders. Sprayed coatings of ball milled powder correspond on average to slightly higher hardness.

Influence of hydroabrasive and electrolyte-plasma treatment on the roughness of heat exchange surfaces manufactured by additive technology

Verbanov I S[@], Lepeshkin A R and Svetlakov A L

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

[@] isverbanov@ciam.ru

The problem of the transition from traditional to additive manufacturing technologies is to reduce the roughness of the external and internal surfaces and choosing the minimum wall thickness of the heat exchanger (HE) channels, which was shown at the previous stages of project development, calculation and construction of additive HE. The previously tested simple mechanical post-treatment of surfaces to reduce roughness showed its inapplicability to internal cavities and hard-to-reach places of complex geometry, and during processing there were characteristic damage to the thin-walled structure up to loss of tightness unacceptable in HE. In order to develop technologies for reducing roughness without loss of tightness, new model samples of branching tree-shaped Ti alloy were made from the heat-resistant alloy CoCrMo and variants of the same design were tested from other promising materials (titanium alloy VT6 and aluminum alloy AlSi10Mg). Regular and experimental technological samples subjected to various targeted post-processing to reduce roughness and passed the most important tests for HE tightness. Shown that it is possible to improve the surface roughness by 2–3 classes—up to 6–8 classes with moderate processing allowances (25–75 μm depending on the material) and maintaining the tightness of the channels, which was confirmed by the tests conducted by the bubble compression method.

Microstructure of TiNiCu melt-spun ribbons crystallized by electropulse treatment

Sitnikov N N[1,2,@], Khabibullina I A[1], Shelyakov A V[2] and Panasova G V[1]

[1] State Scientific Centre of the Russian Federation—Federal State Unitary Enterprise Keldysh Research Center, Onezhskaya Street 8, Moscow 125438, Russia

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

[@] sitnikov_nikolay@mail.ru

This work is devoted to an experimental study of the effect of electric pulse heat treatment on the structure of a Ti50Ni25Cu25 alloy with a shape memory effect. The alloy was fabricated by melt spinning technique from the liquid state in the form of a amorphous ribbon with a thickness around 30 m. The alloy samples were subjected to electropulse treatment (dynamic crystallization) by passing a single electric current pulse with duration of 1–5000 ms through the sample. Electron microscopy and x-ray diffraction studies have shown that electropulse treatment leads to a significant change in the crystalline structure being formed in comparison with the structure obtained by isothermal crystallization. It has been established that after dynamic crystallization the microstructure of the alloys in cross-section has a non-uniform distribution of crystals (grains) over the thickness of the ribbon: a structure of columnar crystals is formed near the surfaces of the ribbon, and individual crystals or grouped large crystals are present in the volume of the ribbon. In additional the columnar structure is characterized by the texture.

The resonant properties of rectangular subwavelength dielectric magnetic dipoles within field of incidence electromagnetic wave of GHz range

Shvartsburg A B[1,@], Pecherkin V Ya[1], Vasilyak L M[1], Vetchinin S P[1], Panov V A[1], Kulikov Yu M[1] and Kostyuchenko T S[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Skolkovo Institute of Science and Technology, Skolkovo Innovation Center Bldg 3, Moscow 143026, Russia

[@] alex-s-49@yandex.ru

The aim of this work was to study the resonance spectra of dielectric rectangles with high relative permittivity for different orientations of the wave vector and the sides of the rectangle. The Agilent E5071C ENA network analyzer was used for generation and registration of the emission spectra of the GHz band. The magnetic field was recorded by a shielded probe with a sensitive circular element with a diameter of 3.8 mm. Magnetic response measurements for a rectangle with dimensions of 20–30 mm and a cross section of 44 mm were performed for different positions of the rectangle plane relative to the wave vector. We carried out experiments for two positions of the rectangle, when the wave vector lies in the plane of the rectangle perpendicular to either the large side of the rectangle or the small side, and the magnetic field vector is perpendicular to the plane of the rectangle. It was found that the frequency of the main magnetic resonance in both positions is the same, and the frequency of the main electric resonance becomes minimal in the case when the large side of the rectangle is collinear with the wave vector. Experimental and theoretical values of resonant frequencies showed a good match. The work was supported by the Russian Foundation for Basic Research, grant No. 18-08-00633.

Resonant interaction of magnetic dipoles in the form of dielectric cylinders in the GHz frequency range

Vasilyak L M[@], Pecherkin V Ya, Shvartsburg A B, Vetchinin S P and Privalov P A

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

[@] vasilyak@yandex.ru

The magnetic interaction of subwave dielectric cylinders in the field of a plane electromagnetic wave of the GHz band is experimentally investigated. Under the influence of the magnetic field of the incident wave and mutual induction in the circuits associated with the circular profile of the cylinder, azimuthal displacement currents are generated, forming magnetic dipoles. The resonance spectra of the system of coupled magnetic dipoles were measured, and the spectral bands of magnetic induction inversion corresponding to negative values of magnetic permeability were found. In the near wave zone, the dependence of resonances on the relative position of the cylinders and the distance between them is shown. On the basic magnetic mode, the structure of dielectric cylinders is a metamaterial.

Spatial structure of the magnetic field of two magnetically coupled dielectric rings at the main resonant frequency

Privalov P A[@], Vasilyak L M, Vetchinin S P, Pecherkin V Ya and Shvartsburg A B

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

[@] petr.priv@gmail.com

The magnetic interaction of two dielectric rings located along the wave vector of a plane electromagnetic wave of the frequency of the GHz band has been studied experimentally and theoretically. Under the action of electromagnetic induction in the magnetic field and mutual induction of the rings, azimuthal displacement currents are generated, forming magnetic dipoles. The spectra of the system of coupled dipoles were measured, and the resonant frequencies and spectral bands of magnetic induction inversion corresponding to negative values of magnetic permeability were found. The spatial structure of the magnetic field of dielectric dipoles placed along wave vector in the same plane with their resonant interaction was obtained. It is shown that the resonant magnetic field is concentrated inside the dielectric rings. The highest value of the magnetic field was registered in the center of the rings. In contrast to the solitary ring, where the magnetic field is weakened outside the ring, on interconnected rings there is an increase in the magnitude of the magnetic field both around the ring closest to the antenna and in the area between the rings. The work was supported by the fundamental research program of the Presidium RAS No. 6 "New approaches to the creation and study of extreme states of matter".

The main magnetic resonance of two magnetically coupled dielectric rings

Pecherkin V Ya[1,@], Shvartsburg A B[1], Vasilyak L M[1], Vetchinin S P[1], Volpyan O D[3] and Churikov D V[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Scientific and Technological Center of Unique Instrumentation of the Russian Academy of Sciences, Butlerova 15, Moscow 117342, Russia
[3] Scientific-Manufacturing Enterprise Fotron-Auto, Malaya Tulskaya Street 45a Korpus 6, Moscow 115191, Russia

[@] vpecherkin@yandex.ru

The main magnetic resonance of 2 planar dielectric rings magnetically coupled to each other was experimentally investigated for the case when the wave vector is perpendicular to the line drawn through the center of the rings. The Agilent E5071C ENA network analyzer was used for generation and registration of the emission spectra of the GHz band. The dielectric rings used in these experiments with a diameter of 16 mm, a cross-sectional area of 3×3 mm^2 and a permittivity of 170 were placed in the same plane with the wave vector. Spectral measurements showed that the frequency of the main resonance of one ring is 2.43 GHz, its half-width is 12 MHz. For two rings, we observed an increase in the depth of the main magnetic resonance and a broadening of the half-width of the resonance line to the root of two, which is associated with an increase in losses in the two rings. This result differs from the case of two rings along the wave vector, in which there is a splitting of resonances, as was previously found in [1].

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On filling the gap of a vacuum-insulated line with plasma

Aleksandrov V V[1], Branitskii A V[1], Grabovski E V[1], Frolov I N[1], Khishchenko K V[2,3], Oleinik G M[1], Samokhin A A[1,@], Shishlov A O[1] and Tkachenko S I[1,2,3]

[1] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia

[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

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

[@] samokhin@triniti.ru

When a high-density current pulse flows via a magnetically insulated transmission line (MITL), a line break is filled with plasma as a result of its ablation from a current-carrying surface. This can lead to noticeable current losses and, consequently, to a smaller contribution of energy to the studied load. To obtain the most extreme parameters in a load in an experiment, the possibility of efficiency increasing of the MITL when coating its current-carrying surface with various materials was investigated. Thin-walled tubes were used as a model of the line node, which is subjected to the greatest dynamic and energy loads. The results of experimental and numerical simulation of the flow of current with a density of about 3 MA/cm along a steel tube ($l = 6$ mm is the tube length, $d = 3$ mm is the tube diameter and $h = 0.5$ mm is the tube wall thickness) are presented, half the length of which was covered with lead foil 180 μm thick or protected by a ceramic layer 700 μm thick. It was found that the rate of expansion of plasma jets from the tube surface to the lead-coated region is 1.5 times lower. It is also shown that in the ceramic-coated region, plasma radiation appears 250 ns later. Thus, when using such coatings, the filling of the MITL gap by the plasma will occur later, therefore, the efficiency of transporting the current to the load will be higher. Estimates of plasma parameters were also obtained at different instants of time.

Electrical explosion of flat conductors in megagauss magnetic fields

Oreshkin V I[@], Chaikovsky S A, Datsko I M, Labetskaya N A, Rousskikh A G and Vankevich V A

Institute of High Current Electronics of the Siberian Branch of the Russian Academy of Sciences, Akademichesky Avenue 2/3, Tomsk 634055, Russia

[@] oreshkin@ovpe.hcei.tsc.ru

The propagation of a nonlinear magnetic-field diffusion wave generated under the condition of an electrical explosion of flat conductors is investigated in the current skinning mode. Using a MIG terawatt generator, a number of experiments are performed on electrical explosion of a copper foil, 100 μm in thickness and 5 mm in width, at the current amplitude up to 2.5 MA and its rise rate 100 ns. It is shown that under these conditions a plasma channel is formed by approximately 75-th ns from the current onset. The estimations, made considering the magnetic field enhancement on the foil edges, demonstrate that about 70–80 ns are required for the nonlinear magnetic-field diffusion wave to propagate from the foil edge to its center. A good agreement of the experimental data and the estimates suggested a conclusion that the plasma channel formation is due to the convergence of the nonlinear diffusion wave towards the longitudinal foil axis.

Intensification of heat transfer during spinodal decomposition of a superheated aqueous oligomer solution

Volosnikov D V[1,@], Povolotskiy I I[1], Igolnikov A A[1], Son L D[3,4], Vasin M G[2,4] and Skripov P V[1]

[1] Institute of Thermal Physics of the Ural Branch of the Russian Academy of Sciences, Amundsen Street 107a, Ekaterinburg 620016, Russia
[2] Institute for High Pressure Physics of the Russian Academy of Sciences, Kaluzhskoe Shosse 14, Troitsk, Moscow 142190, Russia
[3] Ural State Pedagogical University, Kosmonavtov Avenue 26, Ekaterinburg 620017, Russia
[4] Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

[@] dima_volosnikov@mail.ru

The purpose of this work is to study heat transfer in a solution that is overheated by pulses relative to the liquid–vapor and liquid–liquid equilibrium lines. The temperature plateau mode, as a specific case of the technique of controlled pulse heating of a wire probe, was used. The object of the study was an aqueous solution of polypropylene glycol-425 (PPG). In the experiment, the heating power $P(t)$ required for stabilizing the probe at the selected temperature T ($t > t_1$) is measured. The heat flux through the probe surface during the pulse $q(t) = P(t)/S$ is calculated, where S is the probe area. The heat conduction at a chosen time moment is given by $K(t) = q(t)/(T(t) - T_0)$; $K(t)$ is a property both the process and the substance in the relative measurement variant. The position of the liquid–liquid binodal and the coordinates of the lower critical solution temperature are visually determined on the temperature–concentration diagram of the PPG-425–water solution. It has been shown that when spinodal decomposition is realized, instantaneous values of the heat conduction of a solution with a PPG share of 0.1–0.3 exceed the corresponding values for water by 1.5–2 times. This study was supported by the Russian Science Foundation (project No. 19-19-00115).

Theoretical study of ultrafast switching of polarization in ferroelectrics

Starykh E D[1,2,@]**, Zhilyaev P A**[1,2] **and Akhatov I S**[1]

[1] Skolkovo Institute of Science and Technology, Skolkovo Innovation Center Bldg 3, Moscow 143026, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] yelizaveta.starykh@phystech.edu

The spontaneous macroscopic polarization of some tetragonal structured compounds (such as $PbTiO_3$, $BaTiO_3$, etc) gives the opportunity to use these materials in ultrafast non-volatile storage devices [1]. In order to switch the internal polarization, the external electric field must be applied on the certain frequency, which can be derived using the knowledge of chemical composition and crystal structure. In this work we perform first-principle studies of ferroelectric materials with perovskite structures. From the material's phonon spectra we obtain the optically active normal modes, their frequencies and corresponding atomic displacements along each normal mode coordinate. By activating two (or more) normal modes and calculating the energy surface we can obtain the additional unidirectional force due to a nonlinear coupling between two modes [2]. Therefore, we can get the recipe for each individual material to switch the polarization in the fastest and the most effective way possible. The method we use to study ferroelectric properties of the perovskite structures were performed using density functional theory (DFT) implemented in the VASP software package [3].

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Pushing the limits of classical laser flash analysis to advance nuclear fusion research

Lunev A[1,@] **and Aliev T N**[2]

[1] Culham Centre for Fusion Energy, United Kingdom Atomic Energy Authority, Culham Science Centre, Abingdon, Oxfordshire OX143EB, United Kingdom (Great Britain)
[2] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia

[@] artem.lunev@ukaea.uk

Flash laser analysis (LFA), an experimental technique for measuring the thermal properties of condensed matter, is highly regarded for its applicability over a wide temperature range and under extreme conditions associated with radioactive or hazardous materials. Currently, the ASTM standard E1461-13 [1] limits the applicability of the classical method to "essentially fully dense (preferably, but low porosity would be acceptable), homogeneous, and isotropic solid materials that are opaque to the applied energy pulse". The authors challenge that definition and explore heat transfer in non-classical settings, which may include: translucent (semi-transparent) materials with or without opaque coatings; coated diathermic materials; competing heat conduction of a material and its opaque conducting shell, etc, which are subjected to a 0.1–10 ms low-energy laser pulse. The finite-difference solutions of several heat conduction and coupled radiative-conductive heat transfer problems were incorporated in PULsE [2] (processing unit for laser flash experiments), an advanced open-source software toolkit developed at UKAEA for post-processing raw data generated by the LFA instruments. The models have been successfully validated against an array of experimental data for samples conforming to the settings above.

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Recent validation: Express method of WWER-1000 fuel burnup evaluation

Vilkivskaya O V[1,@], Evdokimov I A[1], Likhanskii V V[1], Afanasieva E Yu[1] and Sagalov S S[2]

[1] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia

[2] Joint Stock Company State Scientific Centre Research Institute of Atomic Reactors, Zapadnoye Shosse 9, Dimitrovgrad, Ulyanovsk Region 433510, Russia

[@] vilkhiv@triniti.ru

Accurate evaluation of fuel burnup in case of leaking fuel assemblies (LFAs) manifestation is a challenging issue for modern nuclear power plants (NPPs) [1]. The most sensitive indicator of the leaking fuel burnup in WWER-1000 is the ^{134}Cs-to-^{137}Cs activity ratio at spike-events. A common approach to evaluate the burnup of LFAs was to use a precalcuated dependence of this ratio on fuel burnup. However, analysis of spike events recently showed some discrepancies with this technique. The present work continues the series of papers outlined in [1, 2] focused on the operational conditions in modern fuel cycles and improvement of the existent technique at NPPs. Validation of the proposed models for express burnup evaluation utilizing ^{134}Cs-to-^{137}Cs activity ratios in this report relied on the data for three TVSA that were examined at SSC RIAR, [3]: the results of gamma-scanning of the witness fuel rods in hot cells were used to evaluate ^{134}Cs-to-^{137}Cs activity ratios in fuel, and compare them to the calculated ratios and the available NPPs data on the results of testing in failed fuel detection system casks. A series of validation checks were performed to show that the models reproduce experimental data on caesium activity ratios in fuel of advanced FA designs with a good accuracy. An increased reliability in estimating LFA burnup while performing cladding integrity monitoring at NPPs may be achieved for reactor operation involving spike-events.

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Thermalization of the plasma arising during counter collision of high-energy plasma flows in a longitudinal magnetic field

Gavrilov V V[1], Eskov A G[1], Zhitlukhin A M[1], Kochnev D M[1,@], Pikuz S A[2,3], Poznyak I M[1], Ryazantsev S N[2,3], Skobelev I Yu[2,3], Toporkov D A[1] and Umrikhin N M[1]

[1] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia

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

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

[@] dimich17@triniti.ru

Experimental results on the dynamics and thermalization of plasma formed as a result of the reciprocal interaction of two high-energy plasma flows are presented and discussed. The interaction of the flows occurred in a longitudinal 2 T magnetic field. Nitrogen and neon and their mixtures with deuterium, were used as plasma-forming gases. The dynamics of plasma formation was determined by the signals of magnetic probes, while the dynamics of its electron temperature was determined using photodiodes located behind various filters and registering x-ray plasma radiation. It was shown that in the time interval of 6–8 μs, the electron temperature of the plasma changes insignificantly, i.e., plasma behavior is characterized by quasistationarity. Time-resolved calculations of the ion kinetics were held for nitrogen and neon plasma with the collisional-radiative spectral analysis code. The obtained temporal profile of the x-ray intensity is in a good accordance for the case of neon plasma, but such a good correspondence is not observed for the nitrogen plasma. The reported study was funded by the Russian Foundation for Basic Research according to project No. 18-29-21013.

DD and proton–boron synthesis at the compact scheme of plasma electrodynamic confinement

Kurilenkov Yu K[1,@], Oginov A V[2], Tarakanov V P[1], Samoylov I S[1] and Gus'kov S Yu[2]

[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

[@] kurilenkovyuri@gmail.com

In recent years, we have been investigating, on the basis of nanosecond vacuum discharge (NVD), the not quite usual scheme of inertial electrostatic confinement (IEC) [1]—this is an IEC scheme with reverse polarity [2]. It contains the injection of electrons into the anode space, the formation there of a virtual cathode (VC), created by electrons in the region of their deceleration, and the corresponding potential well (PW). Ions oscillate in the PW, reaching energies up to ~ 100 keV at the moments of head-on collisions. At the collapses of ions at PW "bottom", both DD and aneutronic p + B11 nuclear synthesis take place. The presence of harmonic ion oscillations partially contributes to VC retention also [3]. Therefore, in general, the confinement in our scheme of NVD [2,3], in fact, is more correctly have to be called as electrodynamic (or oscillatory) one. This report presents a review and analysis of the main activity on the reverse-polarity IEC scheme, including our recent results on DD and proton–boron synthesis.

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Diagnostics of focal spot of a linear induction accelerator in the conditions of target plasma distribution

Kolesnikov P A[1,@], Akhmetov A R[1], Chernitsa A O[1], Petrov D V[1], Nikitin O A[1], Trunev Yu A[2], Skovorodin D I[2], Atlukhanov M G[2], Burdakov A V[2], Danilov V V[2], Kurkuchekov V V[2], Popov S S[2] and Zhivankov K I[2]

[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] Budker Institute of Nuclear Physics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 11, Novosibirsk 630090, Russia

[@] kolesnikov.peter@mail.ru

RFNC-VNIITF put the facility based on linear induction accelerator (LIA) into operation in order to study dynamically developing objects due to explosive loading according to pulse x-ray radiography method. One of LIA basic advantages is the high-quality electron beam and small size of a focal spot influencing the accuracy of delimitation of the test subject element. High-energy release in the target because of electronic beam deceleration, leads to formation of plasma torch. Therefore, the focus spot of the second and subsequent LIA gamma pulses increases in the multi-pulse mode. One should be able to determine its parameters and record dynamics of its propagation to search and introduce technical decisions on target plasma neutralization. Thus, it is necessary to monitor a focal spot, which includes explosive experiments, using stationary diagnostic system. This paper presents the research results of the target plasma propagation using method of x-ray probing by the facility, based on a point Z-pinch (Institute of High Current Electronics SB RAS, Tomsk). It also presents the research results on determination of LIA focal spot using diagnostic system in the negative direction of electron movement by "half shadow of the sharp edge" method.

Applied physics at the Laboratory of High Energy Physics of the Joint Institute for Nuclear Research

Baldin A A[1,2]

[1] Joint Institute for Nuclear Research, Zholio-Kyuri 6, Dubna, Moscow Region 141980, Russia
[2] Institute for Advanced Studies "Omega", Lesnaya 3 Office 1, Dubna, Moscow Region 141986, Russia

an.baldin@mail.ru

A unique accelerator complex is under construction at the Laboratory of High Energy Physics of the Joint Institute for Nuclear Research (LHEP JINR). The complex includes the Nuclotron, Booster, and the NICA collider facilities providing accelerated ion beams from protons to gold in an energy range from several MeV/nucleon to several GeV/nucleon. It covers the so called intermediate energy range of relativistic nuclear physics which is of interest in many aspects, including applied research, such as radiobiology, material studies, electronics testing, accelerator-driven-system energy production. The survey of applied research activities at the LHEP JINR is given, special attention is paid to methods and techniques for monitoring and diagnostics of primary and secondary beams. A special Test Zone with secondary beams for applied research and detector testing under construction is presented.

Self-similarity description of relativistic collective phenomena at interaction of high intensity electromagnetic fields with matter

Baldina E G[1]

[1] Joint Institute for Nuclear Research, Zholio-Kyuri 6, Dubna, Moscow Region 141980, Russia
[2] Institute for Advanced Studies "OMEGA", Dubna, Moscow region 141986, Russia

e.baldina@mail.ru

Relativistically invariant self-similarity approach is applied for description of collective particle production and acceleration by femtosecond laser pulses. This approach provides quantitative description of coherent ion production, as well as e^+e^- pair generation under the action of ultrashort laser pulses. This self-similarity approach has proven capable of quantitative description of cumulative, subthreshold, and antimatter production in relativistic nuclear collisions.

Estimation of radioactive impurities in the ^{51}Cr source from photon radiation measurements in the BEST experiment

Gorbachev V V[@], Gavrin V N, Ibragimova T V and Shikhin A A

Institute for Nuclear Research of the Russian Academy of Science, Prospekt 60-letiya Oktyabrya 7a, Moscow 117312, Russia

[@] vvgor_gfb1@mail.ru

The BEST experiment searches for a sterile neutrino state [1]. The activity of the neutrino source ^{51}Cr was measured using γ-ray spectroscopic and calorimetric methods [2,3]. This paper presents the results of the study of photon spectra from the source. The radioactive isotopes and the concentration of elements in the source from which these isotopes are produced in a nuclear reactor are determined. It is shown that the contribution of radioactive isotopes from impurities to the heat release of the source is negligible compared to the heat release of ^{51}Cr. The high purity of the material from which the source is made is confirmed.

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Antineutrino and neutrino satellites of any fissioning process

Shapiyeva A E[1,@] **and Son E E**[2,1]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] shapieva.ae@phystech.edu

The presence of neutron flux coupled with fissioning component like helium-3 isotope creates highly energetic particles at any point of space. Their enormous energy was acquired from transformation of strong interaction energy of fissioning nuclei to kinetic energy of produced particles. Their further evolution can not be resulted by Maxwell distribution due to constant rate of their formation. In addition, each fission fragment has a unique function of energy spectra formed by the inhibitory medium and the energy of the initial fragments. It also should be pointed out that the transformation of strong interaction energy, maintained by gluons, into kinetic energy of fission fragments products can not take place without neutrino or antineutrino participation. Any radioactive decay as well as any nuclear fissioning process is resulting fast particles, among them β-electrons and their immanent satellite antineutrino. Antineutrinos and neutrinos are spreading in all directions and berry all information about what is going on within reactor. In the present paper the typical fissioning process $^3_2\text{He} + ^1_0\text{n} \rightarrow ^1_1\text{p} + ^3_1\text{T} + 0.76$ MeV is analyzed with accent at this problem. This fission reaction is unknown due to variety of all possible transformations of quarks from one type to another. The very high intensity of strong interactions field makes it possible to transform its energy directly to mass creating in this case massive W^+, W^-, Z^0 bosons which start breaking equilibrium within nuclei.

Baksan Underground Scintillation Telescope search for muon neutrinos from the gravitational wave event GW170817

Kochkarov M M[1,@], Boliev M M[1], Butkevich A V[1], Dzaparova I M[1], Kurenya A N[1], Lidvansky A S[1], Novoseltsev Yu F[1], Novoseltseva R V[1], Petkov V B[1,2], Striganov P S[1] and Yanin A F[1]

[1] Institute for Nuclear Research of the Russian Academy of Science, Prospekt 60-letiya Oktyabrya 7a, Moscow 117312, Russia
[2] Institute of Astronomy of the Russian Academy of Science, Pyatnitskaya Street 48, Moscow 119017, Russia

[@] makhti.kochkarov@yandex.ru

Using the data from the BUST (Baksan Underground Scintillation Telescope), we searched for muon neutrinos and antineutrinos with energies above 1 GeV, coinciding with the gravitational-wave event GW170817, which was recorded on August 17, 2017 by the Advanced LIGO and Advanced Virgo observatories. This is a first detection of the new type of events occurring as a result of a merger of two neutron stars in a binary system. A short gamma-ray burst GRB170817A accompanying this event is an evidence of particle acceleration in the source whose precise position was determined by detection of the subsequent optical signal. No neutrino signals were found with the BUST in the interval ±500 s around the moment of the gravitational wave event GW170817, as well as during the next 14 days. The upper limits on integral fluxes of muon neutrino and antineutrino from the source are derived.

Impact of nuclear gluon distributions on leptoquark production by neutrinos

Alikhanov I[1,2]

[1] Institute for Nuclear Research of the Russian Academy of Science, Prospekt 60-letiya Oktyabrya 7a, Moscow 117312, Russia
[2] Institute of Applied Mathematics and Automation of the Kabardino-Balkar Scientific Center of the Russian Academy of Sciences, Shortanova 89a, Nalchik, Kabardino-Balkaria 360000, Russia

ialspbu@gmail.com

We investigate non-standard neutrino interactions with atomic nuclei through leptoquark excitations. A leptoquark term in the Lagrangian admits the possibility that neutrinos interact with gluons. The current lower limits on the leptoquark masses are of the order of 1 TeV depending on the leptoquark quantum numbers and couplings. Such heavy states can be produced in ultra-high energy cosmic neutrino scattering processes. The momentum transfer squared, Q^2, and the Bjorken variable, x, simultaneously probed in these processes may reach values kinematically inaccessible at present collider experiments. We study the impact of the gluon density in a nucleus on the cross section for the leptoquark production by neutrinos. We show that taking into account the nuclear parton distributions shifts the production threshold to essentially lower neutrino energies. As a particular case we consider the interaction with oxygen, which is abundant in water targets used in neutrino detection experiments.

Search for hadronic solar axions

Akhmatov Z A[1]**, Berezin S S**[2]**, Gavrilyuk Yu M**[3]**,
Gangapshev A M**[3,1,@]**, Derbin A V**[4]**, Drachnev I S**[4]**,
Kazalov V V**[3]**, Khokonov A Kh**[1,6,5]**, Kuzminov V V**[3,1]**,
Kobychev V V**[6]**, Muratova V N**[4]**, Panasenko S I**[7]**,
Ratkevich S S**[7]**, Tekueva D A**[3]**, Unzhakov E V**[4] **and
Zavrazhnov A Yu**[2]

[1] Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia
[2] Voronezh State University, Universitetskaya Ploshchad 1, Voronezh 394018, Russia
[3] Institute for Nuclear Research of the Russian Academy of Science, Prospekt 60-letiya Oktyabrya 7a, Moscow 117312, Russia
[4] Petersburg Nuclear Physics Institute named by B. P. Konstantinov of National Research Centre "Kurchatov Institute", Mikroraion Orlova Roscha 1, Gatchina, Leningrad Region 188300, Russia
[5] Kabardino-Balkar Scientific Center of the Russian Academy of Sciences, Inessa Armand 37, Nalchik, Kabardino-Balkaria 360051, Russia
[6] Institute for Nuclear Research of National Academy of Sciences of Ukraine, Prospekt Nauky 47, Kyiv 03680, Ukraine
[7] Karazin Kharkiv National University, Svobody Square 4, Kharkov 61022, Ukraine

[@] gangapsh@list.ru

Resonance excitation of the first nuclear level of ^{83}Kr ($E = 9.4$ keV) by solar axions formed via the Primakoff mechanism and via an M1-transition in the ^{83}Kr nucleus in the Sun is searched. The γ and x-ray photons and the conversion and Auger electrons arising from the excited-level relaxation are detected with a proportional counter in the underground low-background facility of the Baksan Neutrino Observatory. The following experimental constraint is obtained for the product of the axion–photon coupling constant and the axion mass: $|g_{A\gamma} \times m_A| \leqslant 6.16 \times 10^{-17}$. In the framework of the hadronic-axion model, this corresponds to a new axion-mass constraint of $m_A \leqslant 12.6$ eV at 95% of the confidence level (CL). In case of pure hadronic interaction, the upper limit for axion–nucleon coupling is $|g^3_{\mathrm{AN}} - g^0_{\mathrm{AN}}| \leqslant 8.3 \times 10^{-7}$ at 95% CL, which corresponds to upper limit for hadrionic axion mass: $m_A \leqslant 64$ eV at 95% CL with the generally accepted values $S = 0.5$ and $z = 0.56$.

Large-volume detector at the Baksan Neutrino Observatory of the Institute for Nuclear Research of the Russian Academy of Sciences: Detector prototype

Fazliakhmetov A N[1], Gangapshev A M[1,3], Gavrin V N[1], Ibragimova T V[1], Kochkarov M M[1], Kazalov V V[1], Kudrin D Yu[1], Kuzminov V V[1,3], Lubsandorzhiev B K[1], Lukanov A D[1], Malyshkin Yu M[1,2], Novikova G Ya[1], Petkov V B[1,4], Shikhin A A[1], Sidorenkov A Yu[1], Veretenkin E P[1], Voronin D M[1], Ushakov N A[1,@] and Yanovich E A[1]

[1] Institute for Nuclear Research of the Russian Academy of Science, Prospekt 60-letiya Oktyabrya 7a, Moscow 117312, Russia
[2] National Institute for Nuclear Physics, Piazza dei Caprettari 70, Rome 00186, Italy
[3] Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia
[4] Institute of Astronomy of the Russian Academy of Science, Pyatnitskaya Street 48, Moscow 119017, Russia

[@] nikitaushakoff@gmail.com

In the Baksan Neutrino Observatory of the INR RAS (Institute for Nuclear Research of the Russian Academy of Sciences, Moscow), located in the mountains of the Caucasus, it is proposed to create at a depth corresponding to ≈ 4700 mwe (meter water equivalent), a large-volume neutrino detector on the basis of a liquid scintillator with a target mass of 10 kt [1]. This report describes the current state of the first stage of the project, namely a prototype detector with a scintillator mass of 0.5 t. The design of the detector, the equipment and methods used are described.

[1] Sinev V V *et al* 2017 *Phys. At. Nucl.* **80** 446–54

Carpet-3 experiment for superhigh-energy astrophysics: Current-state and prospects

Romanenko S V[1,@], Petkov V B[1,2], Dzhappuev D D[1], Lidvansky A S[1], Gorbacheva E A[1], Dzaparova I M[1,2], Kudzhaev A U[1], Klimenko N F[1], Kurenya A N[1], Mikhailova O I[1], Khadziev M M[1], Troitsky S V[1], Yanin A F[1] and Zhuravleva K V[1]

[1] Institute for Nuclear Research of the Russian Academy of Science, Prospekt 60-letiya Oktyabrya 7a, Moscow 117312, Russia
[2] Institute of Astronomy of the Russian Academy of Science, Pyatnitskaya Street 48, Moscow 119017, Russia

[@] vsrom94@gmail.com

The detection of ultra-high energy cosmic radiation is a unique tool in modern astrophysics. Radiation does not deflect in magnetic fields; therefore, it carries reliable information about the source location that it makes possible to study the spatial distribution of the radiation and its sources. Extensive Air Shower (EAS) arrays are using to register cosmic-rays in the energy range of 10^{14} to 10^{17} eV. Baksan EAS array belongs to such a class. It is preparing at the Baksan Neutrino Observatory, which situated near Mount Elbrus at an altitude of 1700 m above sea level. The main aim of the experiment is gamma-ray astronomy with energy above 10^{14} eV to search for diffuse gamma radiation, sources and study the generation mechanisms of this radiation. The paper provides an overview of the current state of the experiment, as well as prospects.

Spectr-RG–ART-XC: The Universe survey in x-rays

Lutovinov A[@] and Pavlinsky M

Space Research Institute of the Russian Academy of Sciences, Profsoyuznaya 84/32, Moscow 117997, Russia

[@] aal@iki.rssi.ru

The Spectr-RG observatory was successively launched into orbit on July 13, 2019. The Spectr-RG scientific payload includes two x-ray telescopes: eRosita (Germany) and ART-XC (Russia). The both instruments are designed for the all sky survey and detection of the most energetic objects and events in the Universe: clusters of galaxies, active galactic nuclei, neutron stars, black holes as well as transients of a different nature. In the early months of Spectr-RG, the ART-XC telescope observed about half the sky, recorded hundreds of sources with various observational properties: from energy flares on stars to gamma-ray bursts. Here we briefly report on these results.

Neutron stars as a key element of autonomous deep space positioning system

Molkov S[@], Lutovinov A, Arefiev V and Pavlinsky M

Space Research Institute of the Russian Academy of Sciences, Profsoyuznaya 84/32, Moscow 117997, Russia

[@] molkov@cosmos.ru

In this presentation, we give a brief review of neutron star properties and mechanisms of their emission, allowing them to be lighthouses of the Universe. We present concept of autonomous navigation system for spacecrafts in the deep space based on signals from rapidly rotating neutron stars (x-ray pulsars). We show examples of using signals from x-ray pulsars to determine the position of satellites, as well as to calibrate the onboard clock of the Spectr-RG mission, which was launched in 2019.

Hubble's law and microwave cosmic background in the light of the Galactocentric paradigm

Barenbaum A A

Oil and Gas Research Institute of the Russian Academy of Sciences, Gubkin Street 3, Moscow 119991, Russia

azary@mail.ru

Based on the ideas of the galactocentric paradigm [1], it was shown [2, 3] that the Hubble's law and microwave cosmic background can be explained by the interaction of photons with gravitational fields in outer space. Hubble's law and microwave cosmic background are necessary consequences of the subordination of photons in space to the four basic laws of physics: of energy conservation, the constancy of the speed of light, Newton's law of gravity and Planck's law. In this case, the microwave background is the result of thermalization of photons in outer space with the temperature which is determined by the energy of the optical radiation of stars. The transfer of photon energy to the cosmic background and vice versa occurs in accordance with the Planck quantum law.

Two theoretical models are constructed. The first model allows us to obtain a new expression for the value of the Hubble's constant. The second model takes into account the balanced circulation of the Metagalaxy matter, accompanied by the destruction of stars in galaxies and the formation of new young stars from their gas and dust products. Circulation matter is in dynamic equilibrium, at which the energy density released during the synthesis of ^{4}He from hydrogen in young stars and then emitted by them in the optical wavelength range corresponds to the energy density of the cosmic background.

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[2] Barenbaum A A 2018 *Inzh. Fiz.* **6** 18
[3] Barenbaum A A 2019 *Inzh. Fiz.* **1** 31

Arc pyrolysis of methane in the presence of oxygen

Godina E P[1,2,@], Subbotin D I[1,2] and Popov S D[2]

[1] Saint-Petersburg State Technological Institute (Technical University), Moskovsky Avenue 26, Saint-Petersburg 190013, Russia
[2] Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, Russia

[@] godina-ekaterina@mail.ru

Currently, the use of fullerenes is very limited. This is due to its high cost. The main method for producing fullerenes for a long time is the Kretchmer method. This method is based on electric arc evaporation of graphite electrodes in a helium atmosphere. This method has several disadvantages: high electric current, low efficiency, frequent accidents, the use of expensive helium, and a deep vacuum. We have developed a method for the synthesis of fullerene soot from hydrocarbons in an alternating current electric arc plasma torch. Depending on the hydrocarbon used, the content of light fullerenes in soot was from 1.5 to 7% by weight. Such a low yield is associated with the interaction of the synthesis products with hydrogen formed by pyrolysis. In order to remove this hydrogen, oxygen is supplied to the plasma torch. A similar method is used in the synthesis of fullerenes in a laminar flame. The plasma torch used consists of two perpendicular channels made of graphite. On three sides of these channels are graphite rod electrodes. The fourth side is the exit from the electric arc zone. Argon is supplied to the electrode area to prevent soot settling on fluoroplastic insulators. Methane is fed into the arc burning zone. The reaction products are cooled in a water cooler and collected in a cyclone. The resulting carbon black was analyzed by various physicochemical methods: scanning electron microscopy, photon correlation spectroscopy, electron spectroscopy of the extract. It was found that two fractions of soot are formed as a result of pyrolysis. The first fraction, with particles larger than 200 nm, is formed as a result of erosion of graphite electrodes. Soot with smaller particles is primarily formed from hydrocarbons.

Optimization of the process of two-stage pyrolytic conversion of biomass into synthesis gas

Lavrenov V A[@] and Zaichenko V M

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

[@] v.a.lavrenov@gmail.com

The results of heat flow modeling in an setup for two-stage pyrolytic processing of biomass into synthesis gas are presented. The optimal processing mode for a mixture of sawdust and bark (waste from a pulp and paper mill) was obtained, which is characterized by an equilibrium state in which the amount of charcoal formed from biomass is sufficient to meet the setup own needs for thermal energy. The capacity of the experimental setup, taken as the basis for the calculation, is 300 kg/h. The synthesis gas has high purity (less than 50 mg/m^3 of resin and solid particles), a relatively high heat of combustion (11 MJ/m^3) and consists almost entirely of hydrogen and carbon monoxide, which makes it an ideal mixture for the synthesis of liquid chemical products such like methanol, dimethyl ether, gasoline, etc.

A new method for energy gas producing from biomass

Shevchenko A L[1,@], Zaichenko V M[1], Sytchev G A[1], Krylova A Y[1], Madumarova M M[1] and Naletov A Y[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Mendeleev University of Chemical Technology of Russia, Miusskaya Square 9, Moscow 125047, Russia

[@] shev@jiht.ru

This article provides information about new technology for biomass energy utilization developed at the Joint Institute for High Temperatures of the Russian Academy of Sciences (JIHT RAS). Biomass includes peat, wood and agricultural waste, waste products of various kinds. In this case, various types of waste are considered as raw materials for local energy production. Such a statement allows to solve the problems associated with development of local fuel and energy resources energy using and the disposal of various waste types. To date, there are two popular technologies for producing energy gas in process of carbon-containing materials thermal conversion: pyrolysis and gasification. In relation to existing, the developed technology allows to obtain gas with higher efficiency. Reducing energy consumption is achieved through the use of energy released during exothermic reactions, which is accompanied by heating of various types of biomass, which, as it follows from the literature, is realized for the first time in the processes of producing gas fuel. The second energy-saving factor of the developed technology is that the heat source is the gas piston power unit (GPU) combustion products. In this case, a cogeneration scheme is implemented. The results of experiments on the biomass conversion in GPU combustion products and numerical calculations based on a mathematical model that includes the mass conservation equations, energy and balance of chemical elements in a one-dimensional non-stationary approximation are presented. The method of biomass thermal conversion under development will make it possible to obtain gas fuel for energy supply systems at local fuel and energy resources.

Co-combustion characteristics of coal-containing waste and biomass

Faleeva Yu M, 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

[@] sinelshchikov@mail.ru

One of the promising technologies for the disposal of coal waste with high ash content is their co-firing with biomass. Such technologies will make it possible to use a rather high energy potential of coal-containing waste and to reduce the negative impact of the fuel and energy complex on the environment. In the paper two types of coal-containing waste were considered: ash and slag waste of thermal power plants and carbon concentrate obtained by enriching ash and slag wastes. Wood waste were used as biomass. The preliminary measurements showed that the carbon concentrate has a higher fixed carbon content, lower volatile and ash content. Based on the results of thermogravimetric analysis carried out both in flow of nitrogen and air, the combustion characteristics of the feedstock and blends of various compositions were determined. From research results it follows that, despite the significantly different temperature ranges of biomass and coal-containing waste combustion, an influence of the blend composition on the characteristics of its combustion is observed. Biomass additives lead to an evident increase in the reactivity of ash and slag waste with respect to oxidative reactions, which is expressed in an increase in the mass loss rate and a shift of the rate maximum to lower temperatures. With an increase in the biomass fraction in the blend this effect increases. For a carbon concentrate having a markedly higher reactivity compared to ash and slag waste, the positive effect of biomass additives on the combustion characteristics does not appear. It should be noted that biomass additives reduce the carbon burnout temperature for coal-containing waste of both types. This work was financially supported by the Ministry of the Russian Federation for Education and Science (project No. 05.604.21.0232, unique identifier RFMEFI60419X0232).

Characterization of the pyrolysis products of coffee husk and parchment

Faleeva Yu M[1,@], Zaichenko V M[1], Kniazeva M I[2] and Kulikov A B[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] A. V. Topchiev Institute of Petrochemical Synthesis of the Russian Academy of Sciences, Leninsky Avenue 29, Moscow 119991, Russia

[@] faleeva.julia@mail.ru

Coffee is one of the main agricultural commodities in the world and the second export commodity after oil. The nature of the formation of coffee waste depends on the type of processing of coffee beans after harvest. The coffee berries have a complex layered structure. The main byproduct of dry processing is coffee husks (a mixture of all layers) with a yield of approximately 50% by weight of coffee beans. Wet processing includes several steps and allows recovery of the coffee parchment separately from other layers of coffee berry with a yield of approximately 6% by weight of beans. Pyrolysis is the thermal decomposition of materials in the absence of oxygen, which is accompanied by the formation of non-condensable gases, biochar and pyrolysis liquid. This work presents the results of the pyrolysis of coffee husks and parchment at two final pyrolysis temperatures of 350 and 500 °C. Experimental data are presented including composition and quantity of pyrolysis products. Obtained biochar has higher calorific values when compared to raw materials (from 18.2 to 30.7 MJ/kg for husk and from 20.2 to 33.9 MJ/kg for parchment). Pyrolysis gases consist mainly of carbon dioxide, the amount of which decreased with raising temperature (from 73.9 to 61.7% for husk and from 57.0 to 48.3% for parchment). As the pyrolysis temperature increased, gas yield rises from 0.12 to 0.16 MJ/m^3. The liquid analysis shows a change in acetic acid content with increasing temperature (from 62 to 53% for husk and from 30 to 74% for parchment). This reported study was funded by the Russian Foundation for Basic Research, project No. 20-08-00835.

Changes in characteristics of chicken litter torrefaction products during cracking of released vapor-gas mixture

Pudova Ya D[@], Larina O M and Zaichenko V M

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

[@] pudova.y.d@mail.ru

The problem of processing agricultural waste does not lose its relevance. And the ability to utilize waste energetically and thereby use the energy potential contained in them will reduce the environmental damage caused by humanity to nature. To study the effect of pyrolysis processes on various types of biomass, a test bench was created at the JIHT RAS, containing a pyrolysis reactor and a cracking reactor. Thus, as a result of pyrolysis from the feedstock, a vapor-gas mixture is released, which, passing through the cracking reactor, forms synthesis gas. In this work, we conducted a comprehensive study of the effect of low-temperature pyrolysis and further cracking of volatiles on the characteristics of the resulting products (biochar and syngas). The chicken litter was chosen as the studied material. Among the studied characteristics are considered the composition, volume and calorific value of the products. Based on the data obtained, the appropriateness of the process of two-stage heat treatment of the material is assessed. The study was carried out by a grant from the Russian Science Foundation (project No. 18-79-00286).

The study of joint pyrolytic processing of natural and synthetic polymers in solid municipal waste

Egorov K S[1,@] **and Pudova Ya D**[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

[@] blackbird05@mail.ru

As a result of economic development, population growth and urbanization, the amount of municipal solid waste (MSW) accumulated worldwide is growing rapidly. According to forecasts, by 2025 the world annual waste generation will reach 2.2 billion tons. From the point of view of morphological composition, municipal waste is a complex heterogeneous mixture of components, the main fractions of which are natural and synthetic polymers. In connection with the accumulation of a large amount of waste, the solution to the problem of their disposal is becoming increasingly relevant. An alternative way to utilize waste is to use it energetically. Technologies based on thermal decomposition (pyrolysis) have an advantage over combustion due to the closed cycle of the process, which helps to reduce the amount of harmful emissions, does not require expensive fuel preparation and allows the processing of waste of various compositions. Pyrolysis is the thermal decomposition of the organic component of the raw material in an oxygen-free environment, which allows one to obtain a number of products: solid residue, tar, and combustible gas. In the course of the study, the percentage ratio of various types of natural and synthetic polymers in the composition of MSW samples was studied, after which a study was made of the influence of temperature conditions of pyrolysis on the mass yield, composition and properties of products obtained as a result of processing.

4. Methods of Mathematical Modeling

Fate of fragments of the Moon formation during the giant impact

Byalko A V

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

alex@byalko.ru

The most likely scenario for the Moon formation is given by calculations of the giant impact (GI) of the Proto-Earth with a protoplanet with a mass close to Mars. During the GI, gases and silicate fragments with a total mass of about 55% to 70% of the mass of the Moon go to infinity, but infinity for the runaway particles is infinity in the terrestrial reference frame. In the Solar System, these fragments go into finite orbits with periods both less and more than a year. The most important feature of their orbits is that they all pass through the region of the Earth's orbit where the GI occurred. A concentrated gas-dust flow was formed there with a fading intensity; it existed for about a million years. Numerically solving the three-body problem yields numerous fragment trajectories. The probabilities of fragments colliding with the Earth and the Moon are estimated as a function of time after the GI. The most important geophysical consequence of these collisions was the formation of the Earth's atmosphere and the ocean from a concentrated gas and dust stream.

Stable ternary superconducting hydrides in La–Mg–H system

Shutov G M[1,@]**, Kruglov I A**[1,2] **and Oganov A R**[1,2,3]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya 22, Moscow 127055, Russia
[3] Skolkovo Institute of Science and Technology, Skolkovo Innovation Center Bldg 3, Moscow 143026, Russia

[@] shutov.gm@phystech.edu

Inspired by recent works predicting the existence of ternary polyhydrides with promising superconducting properties, we searched for new high-temperature superconductors in the ternary La–Mg–H system. Using evolutionary algorithm USPEX [1–3] and first-principles calculations for crystal structure prediction, we found that well-known hydrides of lanthanum [4,5] and magnesium [6] can form stable ternary hydrides. Two dynamically stable compounds $LaMgH_6$ and La_2MgH_{16} are discovered at 200 GPa, one compound La_2MgH_{12} is found to be stable at 300 GPa and La_2MgH_8 can be stabilized at both 200 and 300 GPa. This work provides diverse properties of these compounds and may give insight into further researches on ternary polyhydrides and ways of their potential synthesis.

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Parameters of the microexplosive cathode processes occurring during the initiation of a vacuum breakdown

Oreshkin E V[1,@], Barengolts S A[2], 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

The report presents the results of numerical simulations of the electrical explosion of cathode microprotrusions initiated by explosive electron emission current. The behavior of the basic parameters of the cathode material (temperature, density, and pressure) during a microexplosion was investigated for copper cathodes. The integral of specific current action has been calculated in relation to the microprotrusion geometry. The formation of a liquid metal fraction during an electrical explosion of a microprotrusion and its motion have been simulated. The parameters of microcraters left by microexplosions on the cathode surface have been calculated.

THERMOS Toolkit: Simulation of non-stationary plasma

Kim D A[@], Vichev I Yu, Grushin A S and Solomyannaya A D

Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, Miusskaya Square 4, Moscow 125047, Russia

[@] dima83ipm@yandex.ru

Modern experimental facilities provide more and more data at high energy densities with one of the distinct feature being very short characteristic times (femto- and picoseconds) of laser interaction with matter. In this case, the rates of elementary atomic processes can be significantly lower than the rate of change of thermodynamic parameters, as a result of which the plasma does not have time to attain equilibrium within the characteristic times of temperature and density change. Modeling of such non-stationary plasma requires solving the system of rate equations at each time step in order to determine the ionic composition and spectral distribution of emission. The THERMOS Toolkit [1] is a software package designed to calculate atomic data and spectral properties of high-temperature plasma, including the capability of non-stationary plasma simulations. In case of dense plasma, the non-stationary rate equations system is solved consistently with ionization potential depression. For these problems a specialized algorithm has been developed for cutting off or adding states of ions at each time step. The presented model of non-stationary plasma has been tested on a number of problems discussed at the Non-Local Thermodynamic Equilibrium (NLTE) and Radiative Properties of Hot Dense Matter International Workshops, which are specializing on NLTE plasma. Comparison of calculation results obtained using THERMOS code with the most advanced codes for cases of non-stationary neon, aluminum, and vanadium plasmas showed good agreement. Calculations have been performed at high performance computer MVS-10P of the Joint Supercomputer Center RAS. The study has been supported by the Russian Foundation for Basic Research, project No. 20-01-00485.

[1] URL http://keldysh.ru/thermos/en/

Seismic barriers filled with granular metamaterials: Mathematical models for granular metamaterials

Kuznetsov S V[1,2,3]**, Morozov N F**[5,4]**, Bratov V**[4,5,@] **and Ilyashenko A**[3]

[1] Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia
[2] Institute for Problems in Mechanics of the Russian Academy of Sciences, Vernadskogo 101-1, Moscow 119526, Russia
[3] Moscow State University of Civil Engineering, Yaroslavskoye Shosse 26, Moscow 129337, Russia
[4] Institute of Problems of Mechanical Engineering of the Russian Academy of Sciences, V.O., Bolshoj 61, Saint-Petersburg 199178, Russia
[5] Saint-Petersburg State University, Universitetskaya Naberezhnaya 7/9, Saint-Petersburg 199034, Russia

[@] vladimir@bratov.com

The problem of seismic protection against the main types of surface acoustic waves and SP (shear–pressure) evanescent waves emanating from vicinity of the epicentre of an earthquake is discussed. The proposed seismic protection method utilized vertical trenches (vertical barriers) filled in with the specially constructed granular metamaterials. Some of the nonlinear hyperelastic models along with nonlinear and inelastic models are analyzed for applications of the usage of granular metamaterials in case of cyclic dynamic loadings that correspond to arrival of the large intensity surface acoustic and evanescent waves. The main attention is paid to arrival of the large intensity Rayleigh, Rayleigh–Lamb and SP waves, as the most frequent waves and most dangerous waves for the engineering structures. Some of the new constitutive equations for metamaterials exhibiting different elastic moduli at tension and compression phases, are proposed and discussed.

Simulation of shock-body interactions using the Runge–Kutta discontinuous Galerkin method with adaptive mesh refinement implemented on graphic accelerators

Korneev B A[1,2,@]**, Zakirov A V**[2] **and Levchenko V D**[1,2]

[1] Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, Miusskaya Square 4, Moscow 125047, Russia
[2] Kintech Lab Limited, 3rd Khoroshevskaya Street 12, Moscow 123298, Russia

[@] boris.korneev@phystech.edu

In this work, we apply a numerical scheme for solving the equations of dynamics of a compressible fluid based on the Runge–Kutta discontinuous Galerkin (RKDG) method [1] and adaptively refined cubic grid (AMR) [2] to the problems of impact interaction with solid and fluid obstacles. Features of effective implementation algorithm for the graphic processor units (GPU) are described. Several well-known validation test problems are considered [3]. Results of full detailed three-dimensional simulations of the shock with the gas or fluid bubble [4] using the developed GPU–RKDG–AMR solver are presented. This work is supported by grant No. 18-71-10004 of the Russian Science Foundation.

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On one method of calculating moving boundaries in Euler coordinates

Shestakovskaya E S[@] and Starikov Ya E

South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia

[@] leshest@list.ru

The paper presents a method for calculating a moving boundary in Euler coordinates as an application to studies of gas flows in areas with an impermeable wall. The method is based on a combination of the Eulerian grid and one Lagrangian border cell formed by the combination of two cells adjacent directly to the moving border [1]. Reconstruction of the entire computational domain is not required. This fact has a significant impact on the computational performance. In contrast to [1], we propose to calculate the internal energy of the combined interval instead of the total energy. We describe the algorithm for combination of cells, present the calculation of thermodynamic parameters, and justify the expression for the internal energy of the combined interval [2]. The method is also generalized to the case of cylindrical and spherical symmetry in the one-dimensional case. The method was verified using an analytical solution to the problem of a converging shock wave in a vessel with an impermeable wall [3]. We show a good convergence of the numerical solution to the analytical one. The proposed method for calculating the thermodynamic parameters of the combined interval does not lead to oscillations of the solution at the boundary. Finally, we compare the entropy functions of the analytical and numerical solutions. Therefore, the developed software package can be used for numerical simulation of technological processes in areas with moving boundaries in Euler coordinates.

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Machine-learning potentials for accurate description of lattice dynamics of complex compounds

Korotaev P Yu[1,2]

[1] Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya 22, Moscow 127055, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

korotaev.py@mipt.ru

The method of automatic construction of interatomic potentials for multicomponent systems [1] is presented. Potentials are trained on the exact energies, forces and voltages calculated in the framework of the density functional theory (DFT). Active learning is used to reduce the number of "expensive" quantum-mechanical calculations and to make the scheme semi-automatic. As a result, only few hundred of DFT calculation are required to "train" interatomic potential, which accurately describes harmonic and anharmonic lattice dynamics. We demonstrate the method on the example of thermal conductivity calculation of Yb-filled skutterudite $Yb_xCo_4Sb_{12}$.

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Ab-initio calculations of point defects in bulk magnetite

Shutikova M I[2,1,@] 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 141701, Russia

[@] shutikova_maria@mail.ru

In order to obtain more accurate data on self-diffusion in magnetite, its defective configurations were investigated in the framework of the theory of the spin density functional. Several types of isolated point defects were treated. Formation and migration energies of the defects were obtained using large supercells and adequate sets of parameters.

The formation of oxygen vacancy is unlikely due to its high formation energy. The formation energy of an interstitial oxygen atom in an octahedral interstitial is 1.44 eV. This value is close to the vacancy formation energy in the octahedral sublattice of iron cations, 1.00 eV, while the vacancy formation energy in the tetrahedral iron sublattice is 2.89 eV.

There are several different types of interstitials that are not occupied in an ideal lattice in octahedral and tetrahedral sublattices, depending on their nearest environment. The result of formation energy for an interstitial iron atom is sensitive to the initial assumption of the magnetic moment of this atom. The formation energies of the interstitials are in range 2.58–5.79 eV.

Xenon bubbles diffusivity in body-centered cubic uranium

Antropov A A[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 141701, Russia

[@] antropov@phystech.edu

There are different mechanisms for the diffusion of bubbles in solids. A classical consideration relates the diffusion coefficient of bubbles with the coefficients of surface and bulk self-diffusion of lattice atoms [1]. The presence of gas in the bubble suppresses surface self-diffusion and diffusion rate of the bubble [2, 3]. However, the diffusion mechanism of faceted nanobubbles can differ significantly from the mentioned above due to the additional energy barrier associated with the formation of terraces on stable faces [4]. Previously, we showed that this factor determines the diffusion rate of empty bubbles in the bcc lattice of uranium. In this work, we consider the effect of gas pressure inside a bubble on the mechanism of a terrace formation on a stable faces using the method of classical atomistic modeling. The directional movement of gas-filled bubbles in bcc uranium is simulated in the pressure gradient [5]. The dependence of the formation energy of the critical step in the face and the diffusion coefficient on the radius of the bubble and xenon pressure is calculated.

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Molecular dynamics study of uranium-dioxide sintering process

Orlova Y V[1,@] **and Kolotova L N**[2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] juliaov00@gmail.com

Uranium dioxide UO_2 has attracted much attention due to its unique nuclear properties and various applications in the nuclear industry. Sintering should be considered one of the major processes in the technological scheme of the oxide nuclear fuel tablets production. Nowadays, there are many works devoted to sintering of uranium dioxide. However, the influence of mutual crystallographic orientation of the particles on the process of pores shrinkage has not been sufficiently studied.

In the present work, we study the process of pores shrinkage during the sintering of UO_2, in particular, the influence of the grain boundary on the rate of this process, using the molecular dynamics method. Computations are performed on 2–4 cylindrical nanoparticles in the conditions of NVE ensemble, with the interatomic potential [1]. Periodic boundary conditions are used to avoid surface effects. We have estimated the surface and grain boundary diffusion coefficients for uranium. The pore shrinkage rate for different crystallographic orientations was measured, and the contribution of the grain boundary to this process was estimated. The influence of the particle size on the sintering rate was studied. The results were compared with the theoretical models represented in [1]. All computations were performed using the LAMMPS package [2].

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Investigation of silicon nanoparticles crystallization

Gordeev I S[1,2,@] and Kolotova L N[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 141701, Russia

[@] gordeevilu@gmail.com

Silicon nano-objects are very interesting for nanophotonics because of their unique optical properties depending on the atomic structure. Their optical properties can be tuned by changing the phase composition and doping by metal atoms. Thus, it is a great interest in study the structural features of these particles, such as the grain size and the distribution of Au and Al atoms in crystal grains and between them. The simulations were carried out in the quasi-two-dimensional case: diameter of nanoparticles (NP) was up to 80 nm and thickness of cell was about 10 nm with periodic boundary conditions. In turn this may result smaller grain sizes in simulation in comparison to the experiment. That is why, additional one-dimensional simulations were performed to study the grain size dependence on the Au or Al concentration in NP. The movement of the crystal grain boundary and changes in the gold distribution during crystallization were analyzed. The influence of cooling rate on Si–Au and Si–Al NP structures was studied in this work for different NP sizes and metal concentrations. The results of simulations indicate that gold atoms try to leave crystallization area via atomic diffusion. So this effect leads to limitation of grain size for larger Au concentrations. The same simulations were carried out for Si–Al NP with developed interatomic potential.

Molecular dynamics study of the properties and structure of the amorphous Zr–Nb alloy

Kliavinek S S[1,2,@] **and Kolotova L N**[2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] klyavinekss@gmail.com

Amorphous alloys are now widely used in applications. Metal glasses have been studied for more than half a century using theoretical, experimental and numerical approaches [1]. Particular attention is paid to studying the structure of amorphous compounds and comparing the results obtained using various methods [2]. In this work, we studied the Zr–Nb alloy. The glass transition process of the supercooled Zr–Nb melt was studied by molecular dynamics modeling. It was determined that the structure of amorphous Zr–Nb consists of interpenetrating icosahedral clusters. The increase in the number of icosahedrons corresponding to a larger number of neighbors is explained by the difference in sizes between the Zr and Nb atoms. It is shown that the splitting of the second peak of the radial-distribution function and the increase in the number of icosahedral clusters in the amorphous structure occur simultaneously. The splitting of the second peak of the radial distribution function is explained through specific distances between atoms in a system of interpenetrating clusters. Using structural criteria, studies of viscosity, diffusion coefficient and elastic modulus, the glass transition temperature was determined for various percentages of Nb. The simulation was carried out using the LAMMPS package [3].

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Microscopic structure and three-particle correlations in liquid and amorphous aluminum

Galimzyanov B N[@] and Mokshin A V

Kazan Federal University, Kremlyovskaya Street 18, Kazan, Tatarstan 420008, Russia

[@] bulatgnmail@gmail.com

Three-particle correlations have a significant effect on various processes occurring in a condensed substance, for example, transport properties in chemical reactions, and amorphization of liquids upon rapid cooling. Experimental methods does not allow to estimate directly of three-particle correlations, whereas detailed information about three-particle correlations can be obtained by molecular dynamics simulation methods.

In this work, we study three-particle correlations in liquid and amorphous Al on the basis of molecular dynamics simulation data. The three-particle correlation function $g(S)$ was introduced to characterize the relative positions of various three atoms (so-called triplets with area S). It was found that in liquid aluminum with the temperatures 1000, 1500 and 2000 K, the three-particle correlations are more pronounced in spatial scales comparable with the size of the second coordination sphere. In the case of amorphous aluminum with the temperatures 50, 100 and 150 K, correlations in the mutual arrangement of the three particles are manifested up to spatial scales that are comparable with the size of the third coordination sphere.

Collective movement behaviour in crystalline and amorphous phases of simple metals

Fleita D Iu[1,3,@], Pisarev V V[1,3] and Norman G E[2,3]

[1] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[3] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] fleyta.du@phystech.edu

The use of correlation functions allows studying simultaneously both microscopic effects (vortex formation and clustering) and the influence of these effects on the thermodynamic behavior. Previously, these features have been studied with the usage of a specific four-point correlation function of the motion in melts of aluminium, nickel and copper with EAM type interaction potentials. It is shown that the crystalline phase is characterized by a higher order of collective motions than in the liquid phase. The effect of an increase in correlations with the crystal heating to the binodal decay is also nontrivial. The particles in unstable positions between the nodes of the crystal lattice show negative correlations. To study the amorphization process, an aluminum film was taken after ultrafast isobaric cooling. Correlation analysis demonstrates motion changes in the characteristic transition region, demonstrating the sharp increase in the consistency of particle motion in the first and second coordination spheres. Estimated glass transition temperature, based on the intersection point of different coordination spheres correlation curves, lies in the region of 570–620 K, which is consistent with other works.

Singularity of the collective behavior in model system in the transition into the metastable liquid

Negodin V D[@], Fleita D Iu, Pisarev V V and Norman G E

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

[@] vdnegodin@gmail.com

We considered a system of particles interacting via Lennard-Jones potential using the method of molecular dynamics. The analysis of particles collective dynamics is presented. We held the detailed examination of the pair correlator behavior near the crystal–liquid transition point in the crossover from stable to metastable state. The correlator characterizes the motion of particles [1,2]; it has the form

$$\mathrm{CC}(T, R, \tau) = \left\langle \frac{[\mathbf{r}_i(t+\tau) - \mathbf{r}_i(t)] \cdot [\mathbf{r}_k(t+\tau) - \mathbf{r}_k(t)]}{|\mathbf{r}_i(t+\tau) - \mathbf{r}_i(t)| \cdot |\mathbf{r}_k(t+\tau) - \mathbf{r}_k(t)|} \right\rangle_{R,t}$$
$$= \langle \cos \varphi \rangle_{R,t}, \quad (1)$$

where $\mathbf{r}_i(t)$, $\mathbf{r}_k(t)$ are the radius-vectors of particles i and k located at a distance R at the initial time, τ is the fixed observation time, and T is the temperature of the system.

Chosen correlator of motion has the singularity of its temperature dependence varying along the isochore. The fracture of correlator is found during the transition from stable to metastable state both by cooling liquid and by melting crystal. The influence of different parameters, such as diagnostic radius and density, is studied. Dependence $\mathrm{CC}(R)$ is in agreement with the radial distribution function and exhibits crystal structure in more sensitive way.

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Singularity at the point of transition from equilibrium to metastable states of Lennard-Jones vapor and liquid

Polyachenko Y A[1,2,@]**, Fleita D Iu**[2,3]**, Pisarev V V**[2,3] **and Norman G E**[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 141701, Russia
[3] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

[@] polyachenko.yua@phystech.edu

This study is devoted to the study of the collective motion of particles in the Lennard-Jones system. A wide range of parameters is analyzed near the liquid–gas coexistence curve. Particle interaction is described by well known Lennard-Jones potential. Periodic boundary conditions are used. Collective dynamics analysis is conducted near the liquid–gas transition region in both directions via pairwise space–time correlators [1]. Presence of a singularity in the isochoric temperature dependence of the correlator [2] $CC(T, R) = \langle \cos (\varphi) \rangle_R$ is shown. Here $\langle \ldots \rangle_R$ is the averaging over pairs of particles initially approximately R apart, $\Delta \vec{r_i}$ is the displacement of i-th particle, φ is the angle between displacements of particles, T is the temperature of the system. Singularity found near the transition point holds for both evaporation and condensation. Dependence of the correlator on a number of parameters such as size of a system, time of particles displacement, initial distance between particles, thickness of the averaging layer is studied. Physical nature of the found effect as a forerunner of the nucleation process is discussed.

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Graphics-processing-unit algorithm for molecular-dynamics simulations with 4-point water model in the LAMMPS code

Nikolskiy V P[1,2,@] **and Stegailov V V**[2,1]

[1] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] thevsevak@gmail.con

Three-point water models are simple and intuitive, but they have a number of disadvantages when used in classical molecular dynamics. Adding a massless virtual charge to each water molecule can significantly improve the distribution of electrostatic fields and makes it possible to model water in a wide range of parameters [1–3]. Such a four-point model TIP4P is more difficult to program and compute. The adaptation of the implemented in LAMMPS TIP4P central-processing-unit code for calculations on graphics accelerators (GPUs) is associated with some difficult problems [4, 5] and could not be done yet. In this work, a new algorithm was created for calculating TIP4P as part of the universal package of classical molecular dynamics LAMMPS. The code was implemented in the GPU module as a pair style `lj/cut/tip4p/long/gpu`. It completely inherits the interface of the standard `lj/cut/tip4p/long` and it is compatible with the `pppm/tip4p`. The code allows the use of Nvidia and AMD GPUs. The new code reduces the time to solution by about 60–70% on typical systems and makes it possible to solve new problems. This work was supported by the Russian Foundation for Basic Research, project No. 18-37-00487.

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Development of the wave packet molecular dynamics and density functional theory method for non-ideal plasma simulations

Lavrinenko Ya S[1,2,@], Morozov I V[1] 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 141701, Russia

[@] lavrinenko@phystech.edu

We report upon development of the wave packet molecular dynamics and density functional theory (WPMD-DFT) simulation technique proposed earlier for nonideal plasma and warm dense matter simulations [1]. The method is based on the WPMD, where the electron exchange-correlation effects are taken into account using the DFT approach. It allows to improve the results for thermodynamic properties at high plasma densities, study simultaneous dynamics of electrons and ions, obtain electron–ion relaxation rates, plasma conductivity and reflectivity. At the same time the WPMD-DFT method is less time consuming than the antisymmetrized WPMD or the path integral Monte-Carlo methods. In this report, we discuss

- special type of boundary conditions that prevent wavepacket spreading and their influence on simulation results;

- usage of graphics processing unit computing and adaptive mesh for calculation of the exchange-correlation energy;

- simulation results for the dense hydrogen plasma in a wide range of temperature and densities;

- preliminary results for the deuterium Hugoniot curve compared with other *ab initio* simulations and experimental data.

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Mathematical modeling of radio-frequency plasma flow at low pressures in non-local approximation

Shemakhin A Yu[@] and Zheltukhin V S

Kazan Federal University, Kremlyovskaya Street 18, Kazan, Tatarstan 420008, Russia

[@] shemakhin@gmail.com

Radio-frequency (rf) plasma at low pressures ($p = 13.3$–133 Pa) with gas flow is effectively used for modifying the surfaces of materials [1]. This type of plasma has the following properties: degree of ionization is 10^{-4}–10^{-7}, electron density is 10^{15}–10^{19} m^{-3}, the electron temperature is 1–4 eV, the temperature of the atoms and ions in the bunch $(3$–$4) \times 10^3$ K in the plasma jet $(3.2$–$10) \times 10^2$ K. The main feature of rf plasma flow at low pressure is that for neutral component plasma flows in a transitional mode between the continuum mode and free-molecule flow, the charged components can be approximated as continuous medium [2, 3]. Mathematical model of rf plasma flow at low pressure in non-local approximation 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 argon and the electron density, electron temperature, electric field are obtained. The reported study was funded by the Russian Science Foundation, research project No. 19-71-10055.

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Stability limits of liquid and gas phases of methane–ethane mixture

Lenev D Yu[1,2,@] and Pisarev V V[2,3]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[3] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

[@] lenevdy@mail.ru

Retrograde condensation is a phenomenon that makes it difficult to produce natural gas from wells. Pressure of the natural gas falls while field development and the mixture reaches retrograde region of phase diagram. It creates an obstacle to extracting gas. The goal of this work is finding a way to dynamically model retrograde condensation and find its kinetic borders. A mixture of methane and ethane is studied with the use of the TraPPE-UA force field. The Nose–Hoover thermostat and barostat are used to keep temperature and pressure constant. Two types of models are considered. First, the mixture is kept at low pressure in the beginning. Then, simulation box is made smaller to create supersaturation. Second, the mixture starts at high pressure. After that, the volume is increased to make the mixture evaporate. The stability limits and the phase diagram are calculated for 250 K. Qualitative agreement with theory is achieved. This means that first the coexistence line and then the stability limit is reached. Both phase diagram and stability limits are also obtained using the Brusilovsky equation. The critical points, calculated using the TraPPE-UA and the Brusilovsky equation, differ and that is why there is no quantitative agreement. The reason for this difference is the interatomic interaction potential, which is used in this study.

Molecular dynamics analysis of entanglements topology in polymer nanocomposites with carbon nanoparticles

Logunov M A[1,2,@] and Orekhov N D[2,1]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] mikhail.logunov@phystech.edu

The properties of polymer nanocomposites differ from those of pure polymers. Addition of the geometrically modified nanoinclusions to the polymer melt has an affect on the mobility of polymer molecules and creates additional topological limitations. The mechanical properties of the model system of a polyethylene matrix with carbon nanoinclusions (nanotubes and graphene surfaces) were investigated within the method of molecular dynamics. The method of calculating the primitive path [1] was used to analyze the change in the topology of the entanglements of the polymer chains during uniaxial deformation for both systems—the pure polyethylene and the nanocomposite. It has been demonstrated that the presence of geometrically modified nanoparticles slows down the process of disentangling. Analyzing the data, an attempt is made to find the connection between the changes in elastic properties and the pore formation [2] arising from the addition of nanoparticles dynamics and the process of disentangling interchain kinks.

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Mechanisms of liquid fiber formation: Experiment and numerical modeling

Kravchenko I V[1], Poldushov M A[3], Miroshnikov Yu P[3] and Patlazhan S A[2,1,@]

[1] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia
[2] Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, Kosygina Street 4, Moscow 119991, Russia
[3] MIREA—Russian Technological University, Vernadskogo Avenue 78, Moscow 119454, Russia

[@] sapat@yandex.ru

Conditions of liquid fibers formation during flow of diluted emulsions in the channel with the sharp contraction were studied experimentally and numerically. The novelty of this study was in determining the role of steric constraints of the channel walls (confinement) upon microfiber formation. For this purpose, a transparent cell was designed to study the emulsion flow at a given pressure drop. Viscosity ratios of castor oil droplets to PDMS (polydimethylsiloxane) matrix were adopted as 0.56 and 5 at the interfacial tension of 4–6 mN/m. It was found that droplets were stretched at the inlet to the narrow part of the channel while the increase in pressure drop results in nonlinear growth of the fiber length. The elongation of the small droplets was significantly less than that of those commensurate with the capillary cross-section. Mathematical modeling was fully consistent with the experimental results and proved that capillary walls strongly influence to the elongation degree of the coarse droplets.

Mixing in droplet co-flowing with Newtonian and shear-thinning fluids

Roshchin D E[1,3,2]**, Kravchenko I V**[2]**, Vagner S A**[2] **and Patlazhan S A**[3,2,@]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, Russia
[3] Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, Kosygina Street 4, Moscow 119991, Russia

[@] sapat@yandex.ru

Mixing processes of two miscible fluids inside a microdroplet flowing along with immiscible Newtonian or shear-thinning media in two-dimensional straight channel were studied numerically. To this end, the system of Navier–Stokes equations for incompressible fluids together with continuity and transport equations for each phase were solved using the open integrable platform OpenFoam. The current position of the interface of the external droplets was fixed by the volume-of-fluid method. The rheological behavior of the shear-thinning fluid was described by means of the Carreau–Yasuda model. The quality of mixing in droplet was estimated by concentration standard deviation from the average value. The influence of the channel width, rheological properties of external fluids, and average flow rate has been studied. It was found that decrease in channel width results in the intensification of miscible fluids mixing in a droplet. This tendency correlates with growing of the inner vortices, which in turn increase the convective mass transfer in a droplet. The replacing of Newtonian liquid by the shear-thinning fluid leads to a noticeable reduction in mixing efficiency in narrow channels, while an increase in Peclet number decreases the mixing time. This work was supported in part by the Russian Foundation for Basic Research (grants No. 18-53-15013) and the Russian Academy of Sciences (RAS, projects No. 0082-2014-0013 and 0089-2019-0001). Numerical calculations were carried out on the computing resources of the Joint Supercomputer Center RAS.

Formation of Newtonian droplets co-flowing with polymeric fluid: Experiment and numerical simulation

Vagner S A[1,@]**, Funfschilling D**[2]**, Serra C**[3] **and Patlazhan S A**[1,4]

[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 Strasbourg, CNRS UMR 7357, Rue Boussingault 2, Strasbourg 67000, France

[3] Charles Sadron Institute CNRS UPR 22, Rue du Loess 23, Strasbourg 67034, France

[4] Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, Kosygina Street 4, Moscow 119991, Russia

[@] vagnerserge@gmail.com

The formation of monodispersed microdroplets is very important for medical and biological applications. An efficient way to generate monodispersed microdroplets is the joint flow of two immiscible liquids through coaxial capillaries. We studied both experimentally and numerically the effect of the rheological properties of the continuous phase on the dynamics of the formation of Newtonian droplets. As the dispersed and continuous phases, silicon oil and shear thinning aqueous solution of peroxyacetic acid (PAA) were used, respectively. The droplet size was found to grow notably as compared to the corresponding dimension of a droplet generated in the co-flowing Newtonian continuous phase. It is almost independent on the flow rate of non-Newtonian fluid, which is significantly different from the corresponding dependence for the couple of Newtonian fluids. These features were explained to cause by the inhomogeneous distribution of the local viscosities of the shear-thinning fluid around the droplet. This study was supported by grants from the Russian Foundation for Basic Research and CNRS No. 18-53-15013 and the Russian Academy of Sciences (RAS) No. 0082-2014-0013 and 0089-2019-0001. The calculations were performed on the computing resources of the Joint Supercomputer Center RAS.

One-dimensional compositional modelling of oscillatory two-phase flow regime in porous media of binary hydrocarbon mixture

Zakharov S A[1,2,@]**, Pisarev V V**[1] **and Chudanov 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 141701, Russia

[@] stepan.zakharov@phystech.edu

An analytical and numerical description of two-phase flows in a porous medium for the one-dimensional case is presented. This research is aimed at modeling of natural gas condensate flows at hydrocarbon reservoir conditions. We focus on examining of a self-oscillatory regime obtained experimentally [1].

Our model is component-scalable, uses generalized cubic equation of state (EOS) [2] and assumes equal pressures in coexisting phases. It can be used for miscible and immiscible fluid in a unified way. The model consists of hydrodynamic equations with respect to densities of components in two-phase state. Filtration processes are described by Darcy's relation with relative permeability functions. We assume local thermodynamical equilibrium which we calculate after computing hydrodynamic time step. To calculate the equilibrium, we apply the VT-flash solver [3] adapted to the generalized EOS. We provide first results for binary mixture flows of alkanes including evoking of liquid holdup and self-oscillatory regime.

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On evaluation of combustion efficiency in a solid fuel ramjet combustor

Razmyslov A V[@] and Sultanov V G

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

[@] sanaraz@mail.ru

In present work, computational fluid dynamics was employed to investigate some features of performance of a typical solid fuel ramjet combustor (SFRJ). Namely dependence of combustion efficiency on fuel grain length. It was shown that combustion efficiency at the outlet of a typical cylindrical SFRJ combustion chamber with length of 50 cm decreases with increase of fuel grain length while combustion efficiency at the grain outlet does not vary significantly after grain length is long enough being circa 0.4 for polyethylene (PE) combustion and 0.2 for hydroxyl-terminated polybutadiene combustion. Total thermal power yield from combustion grows drastically with increase of grain length from 20 to 40 cm, then it does not changes significantly and may even drop due to combustion inefficiency. Performance of PE and hydroxyl-terminated polybutadiene in SFRJ combustor is similar in terms of thermal power yield, while consumption rate of PE is much lower and combustion efficiency is, in general, higher.

Methods of computational and experimental study of icing of elements of an aircraft

Kirilyuk V A[1,2,@] **and Grebenkov S A**[1]

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

[@] kiriluk.94@yandex.ru

The work is devoted to the problem of preparing aviation for operation in difficult weather conditions of icing. The paper describes a computational and experimental method that is universal for researching the work of various elements of aircrafts (engine fairing, aircraft wing, helicopter blade, etc) during icing and is used for their certification. To obtain reliable information about the operation of an element in icing conditions, it is necessary to create a model, whose behavior in a two-phase flow on the test facility most accurately reproduces the behavior of the element in question as part of an aircraft in flight conditions in an atmospheric cloud containing supercooled water droplets. To simulate icing conditions, it is necessary to ensure that the object and its model are geometrically matched and that the flow fields are similar. In this case, the process of forming ice growths on the surface of the test model will occur in the same way as it occurs on a full-size object in flight conditions. The computational and analytical part of the method consists of a set of single-phase and two-phase calculations of the flow of models of the studied objects in modern software systems, which allow to determine the physical parameters that must be maintained on the experimental object for accurate simulation of the test mode. Calculations of the masses and geometries of ice growths on the surfaces of the studied elements are also given, which allow us to identify the most dangerous modes from the point of view of icing. The results of calculations and experiments were verified for some examples. The method allows you to significantly reduce the time of expensive tests on the test facility.

Nucleation of soot nanoparticles from polycyclic aromatic hydrocarbon precursors

Potapov D O[1,2,@] and Orekhov N D[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 141701, Russia

[@] potapov.do@phystech.edu

A comprehension of the mechanism of soot formation is crucial for reducing harmful emissions during combustion, as well as for the synthesis of fullerenes and other carbon structures. It is widely accepted that carbon nanoparticles clusterization process comes through an intermediate stage of formation of polycyclic aromatic hydrocarbons (PAH), but however precise conformational properties of this nanoparticles in the early stages of reaction and nucleation mechanism are still unknown. This work presents analysis of nucleation kinetics of soot particles formed from large PAH structures with more than 60 atoms. Reax force field [1], is selected for molecular dynamics simulations at temperature ranging from 2500 to 3500 K. Structural properties of soot nanoparticles are examined by comparing parameters such as graphitization and hybridization under various thermal conditions.

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Calculating accommodation coefficients in soot structures formation

Goldshtein K D[1,2,@] **and Orekhov N D**[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 141701, Russia

[@] kgoldm19@gmail.com

Soot formation is an important process which affects fuel combustion and synthesis of carbon structures. The formation and growth of soot structures are dependent on the conditions of the process, but the exact mechanism has not been understood well [1, 2]. Using molecular dynamics methods, we focus on the dependence of soot structures growth on temperature in 1500 to 3000 K temperature range. This way, we calculating accommodation coefficients between soot structures obtained from PAHs (polycyclic aromatic hydrocarbons) and a PAH itself. The soot structure surface morphology was also examined. The study provides better understanding of the kinetics of soot structures grow, which is the main objective of our research. The results were obtained using LAMMPS with ReaxFF [2] potential.

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The thermal stability of nascent soot clusters

Shadymov V A[1,2,@] **and Orekhov N D**[1,2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] vladimir.shadymov@gmail.com

The process of fuel combustion and carbon material synthesis are accompanied by the formation of incipient soot particles. Depending on the pathway of soot formation, a different morphology of carbon structures is obtained [1]. In this work, the results of molecular simulation with reaxff potential [2] of soot formation from polycyclic hydrocarbons at high temperatures is observed. Specifically, we focus on such a morphological aspect as the energy required to soot sublimation. The direct calculation of such energy through thermal decomposition in molecular dynamics is computationally demanding. The main objective of our research is to understand the dependence between nanostructure assembly and its sublimation temperature.

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5. Physics of Low Temperature Plasma

Distribution function of the ion microscopic field in a strongly coupled ultracold plasma: Method of molecular dynamics

Zelener B B[@], Bobrov A A, Bronin S Ya, Klyarfeld A B, Zelener B V and Korchagin D S

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

[@] bobozel@mail.ru

Results of calculations of the distribution function of the ion microscopic field at the neutral point of ultracold plasma by the molecular dynamics method are presented. The calculations are carried out for the model of a two-component fully ionized ultracold plasma in a wide range of Coulomb coupling parameter. To evaluate the accuracy of the calculations, the distribution function of the ion microscopic field of randomly distributed charged particles at various concentrations was calculated in order to compare with the exact Holtsmark function. Results obtained for our model can be used for any equilibrium or non-equilibrium strongly coupled plasmas, in which quantum effects are negligible. Comparison with numerical calculations of other authors is made. The work was supported by the Council of the President of the Russian Federation for Support of Young Scientists and Leading Scientific Schools, project No. MD-2189.2019.2. The calculations were performed at the Joint Supercomputer Center of the Russian Academy of Sciences.

Optical spectroscopy of ultracold calcium plasma

Vilshanskaya E V[1,2,@]**, Saakyan S A**[1,4]**, Sautenkov V A**[1,5]**, Bobrov A A**[1] **and Zelener B B**[1,2,3]

[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] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia
[4] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia
[5] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

[@] eva.villi@gmail.com

Our research is devoted to study of ultracold of Rydberg atoms and ultracold nonideal plasma obtained by laser cooling and trapping of neutral atoms in a magneto-optical trap [1, 2]. Recently the two-photon spectroscopy was applied to measure the energies of Rydberg transitions in the n^1S_0 state of ^{40}Ca atoms at $n = 40$–120 and the ionization potential was determined as $49\,305.919\,66(4)$ cm^{-1}. Calcium atoms have two valence electrons. After photoionization, there will be a single valence electron in every ion and strong optical transitions can be observed. It can be used for the optical spectroscopy of non-ideal plasma. In our experiment, a setup for ionization of neutral calcium atoms was assembled. Ion registration is made using the two continuous-wave resonant laser beams with a wavelength of 397 and 866 nm were used. An image of cloud of the ultracold ions was recorded by a CCD (charge-coupled device) camera.

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Optical dipole trap for cold lithium-7 atoms

Saakyan S A[@], Sautenkov V A and Zelener B B

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

[@] saasear@gmail.com

In modern physics the optical dipole trap is a powerful tool to study assembles of ultracold atoms [1]. We present experimental results obtained with our setup for laser cooling and trapping lithium-7 atoms in far-off resonance optical dipole trap [2]. Parameters of the trap such as size of the cold atomic cloud, dipole potential depth and trap losses are investigated. Approximately 3×10^7 atoms are loaded in our dipole trap with the temperature 0.55 mK. The atomic cloud temperature is comparable with the trap depth. In our setup the trap potential is estimated as $U_0/k_B = 0.9$ mK (k_B is the Boltzmann constant). By using fluorescence imaging technique the trap losses induced by modulation of the trap depth are studied. We observe and study superharmonics in the trap loss spectrum. This work was supported by the Russian Science Foundation under project No. 19-72-00099.

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Calculation of the dynamic characteristics of an ultracold resonantly excited gas with a dipole–dipole interaction by the molecular dynamics method

Vikhrov E V[@], Bronin S Ya, Zelener B V, Klyarfeld A B and Zelener B B

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

[@] vikhrov.e@gmail.com

Media with a dipole interaction of particles with randomly oriented dipoles are intensively studied by experimental and numerical methods. The main attention is paid to studying the behavior of ferromagnetic materials in nonmagnetic liquids. The performed studies demonstrate the presence of a first-order phase transition in such systems. At the same time, there are other media in which the interaction of electric dipoles is essential. Such, in particular, are ultracold gases of resonantly excited atoms. This work presents the results obtained by the molecular dynamics method. A program has been developed for calculating the dynamics of processes and transport properties in a gas model of resonantly excited Rydberg atoms. The process of establishing thermodynamic equilibrium and the formation of structures are modeled. A version of a system with equally oriented dipole moments is considered. The pressures and temperatures for a number of points in the phase diagram are determined. For these points, temporary correlation functions are constructed that characterize the change in the correlation maximum with time. It is shown that the characteristic time for the formation of filament structures under the considered conditions is $\sim 10^{-7}$ s. These calculations are necessary to determine the experimental conditions under which phase separation can be observed. The work was supported by the Russian Science Foundation (grant No. 18-12-00424).

Cooling rates for positively and negatively charged ions propagating through ultracold gas of magnetized electrons

Bobrov A A

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

abobrov@inbox.ru

The results of molecular dynamics modeling of the cooling of negatively and positively charged ions in a dense ultracold gas of magnetized electrons are discussed. Single ion with a charge of $-e$ or $+e$ propagating through the electron gas in a cubic simulation cell is considered.The research is aimed to the study of the dependence of the cooling rate on the charge sign of the propagating particle.
The dependence of the cooling rates on angle between the ion velocity and the uniform magnetic field direction is studied. The reference simulations for zero magnetic field are also performed. The calculation results are compared with the previous studies [1, 2].

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Plasma screening enhancement of thermonuclear reaction rates

Chugunov A I

Ioffe Institute, Polytekhnicheskaya 26, Saint-Petersburg 194021, Russia

andr.astro@mail.ioffe.ru

Plasma screening can significantly increase the speed of thermonuclear reactions. The most pronounced effect takes place in the white dwarf cores and neutron star envelopes, there the enhancement factor can be as large as tenths orders of magnitude. Here the thermodynamically consistent description of this effect, which do not lead to violation of the detailed balance principle is discussed.

Optical-polarization properties of nonideal 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

The presence of substantial difficulties in the theoretical description of dense plasma with strong particle interaction leads to the need to obtain as much experimental information as possible on the optical and transport properties of such a medium. The study of the optics of a dynamic object is a powerful research tool, since the optical properties are very sensitive to changes in the electronic subsystem of the medium.

The results of new experiments on reflectivity of polarized light on explosively driven dense xenon plasma are presented. The dependence of the reflective characteristics of a shock-compressed strongly nonideal inert gas plasma on its thermodynamic parameters was studied in the near infrared using a pulsed two-stage YAG laser operating in the Q-modulation mode and a high-speed four-channel polarimeter. The hydrodynamic method traditionally used in the IPCP RAS was used to generate the required plasma states. During the experiments, the plasma density up to $\rho = 1.3$ g/cm^3, pressure up to $P = 6$ GPa and temperature up to $T = 34\,000$ K were realized. Under these conditions, the plasma is non-degenerate. The reflection indexes of a strongly nonideal inert gas plasma were calculated on the basis of the numerical solution of the field equations. The generalized Drude formalism was used to construct the permittivity function of the medium. Thermodynamic parameters of shock compressed plasma were determined using the SAHA IV package [1].

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Asymptotic behavior of the spectral energy distribution of the equilibrium radiation in ideal gaseous plasmas and degenerate electron gas

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

[@] satron@mail.ru

It is shown that the difference between the Planck distribution and the spectral energy distribution of equilibrium radiation in a homogeneous and isotropic material medium is completely determined by the transverse dielectric constant of the material medium. In contrast with the well known approach for the generalized spectral energy distribution of the equilibrium radiation in plasma medium based on the accounting only the frequency dependence of the dielectric permittivity, the crucial role of both frequency and spatial dispersion of the transverse dielectric permittivity is demonstrated. On this basis, the high-frequency and low-frequency asymptotical properties of the spectral energy distribution in an ideal gaseous plasma and degenerate electron gas are considered. The obtained results for the equilibrium spectral distribution are principally different from the corresponding asymptotic of the Planck distribution, possessing a long tail at high frequency and logarithmical increase at low frequency [1–7].

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The thermophysical properties of low-temperature lead 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

Studies of the thermophysical properties of matter (pressure, internal energy, etc, as well as electron transport coefficients) have been going on for more than a century due to their importance for various fundamental problems and applications. There are also corresponding calculations and measurements data for the low-temperature plasma of some elements at the temperatures $T = 10$–100 kK [1]. For Pb (lead), however, there is shortage of corresponding data in this area. At $T \geqslant 10$ kK there are the data of measurements and calculations at relatively high densities [2,3]: at $\rho \geqslant \rho_c$, where $\rho_c \approx 3$ g/cm^3 is the critical point density. At lower densities there is only the research [4], considering the electrical and thermal conductivities. Evidently, this situation should be corrected.

To do it, we have used previously developed model for the considered properties in this area, which has been successfully used for different elements (see [5] and references therein). This model was modified to apply it to the low-temperature partially ionized plasma of Pb [6]. Simultaniously with our investigations the new measurements [7] have appeared. The comparison of our data with the experiments has shown good agreement.

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Electrical conductivity in dilute colloid electrolytes

Shikin V B[1,@] **and Chikina I**[2]

[1] Institute of Solid State Physics of the Russian Academy of Sciences, Akademika Osipyana Street 2, Chernogolovka, Moscow Region 142432, Russia
[2] Interdisciplinary Laboratory on Nanoscale and Supramolecular Organization, Nanoscience and Innovation for Materials, Biomedecine and Energy, CEA, CNRS, Universite Paris-Saclay, Centre d'Etudes de Saclay Bâtiment 125, Gif sur Yvette 91191, France

[@] shikin@issp.ac.ru

We discuss the mechanism of the influence of the multiply-charged colloidal clusters on linear electric transport in diluted polyelectrolytes. The structure of these colloids has well known form—so called DLVO (Derjaguin–Landau–Vervey–Overbeek) clusters. They are effectively neutral and cannot participate in the transfer of charges in the solution. Nevertheless, there is a linear increase in the conductivity of colloidal polyelectrolyte with an increase in the density of colloids $n^\star$. This phenomenon is observed experimentally. It is shown that this happens due to the change of electric field in the polyelectrolyte under the effect of colloidal particle polarization.

Lefschetz thimbles and Wigner functions

Filinov V S[@] and Larkin A 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 main difficulty for the Path Integral Monte Carli simulation of the quantum systems of particles is so called 'sign problem'. However nowadays this term is used to identify two different problems.

The first one arise form from the requirement of antisymmetrization of the matrix elements of the fermion density matrix. To avoid the 'sign problem' it has been derived an effective pair pseudopotential in phase space, accounting for Fermi statistical effects. The derived pseudopotential depends on coordinates, momenta, and the degeneracy parameter of fermions and takes into account Pauli blocking of fermions in phase space.

The second type of the 'sign problem' arises in the Feynman path integral formulation of quantum mechanics and finite density quantum chromodynamics (QCD), where a strongly oscillating complex action does not give a real and positive Boltzmann weight to resort to the traditional Markov chain Monte Carlo methods to estimate quantum averages. There have been many proposals to circumvent the sign problem. One of the approaches that are currently under intense study is the use of integration over Lefschetz thimbles, which is called as the Lefschetz thimble algorithm. There, the original real-valued variables are complexified according to the antiholomorphic gradient flow.

A goal of this work is to find new effective methods for numerical simulations of path integrals with a sign problem as these methods can also provide a new perspective on semi-classical methods in path integration and new approach to semi-classics. Our aim to find techniques of universal character, providing insights to this problem. The ideas from mathematics come from Picard–Lefschetz theory and a complex version of Morse theory

Asymptotics of quantum momentum distribution functions in thermodynamic equilibrium

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

[@] alexanderlarkin@rambler.ru

The object of this work is quantum system of particles with potential interaction $U(q) = kq^\alpha$ with different values of α in thermodynamic equlibrium. Analytical method for calculating quantum momentum distribution function $F(p)$ in the limit $p \to \infty$ is proposed. The basic ideas of this method are as follows. Firstly, the momentum distribution function should be expressed through Wigner function of the canonical ensemble:

$$F(p) = \int_V dq W(p,q), \quad W(p,q) = \int_{-\infty}^{+\infty} d\xi e^{ip\xi/\hbar} \rho\left(q - \xi/2, q + \xi/2\right).$$

Secondly, the density matrix should be represented in form of path integral with the given boundary values $q(\pm\hbar/2kT) = q \mp \xi/2$:

$$\rho\left(q - \xi/2, q + \xi/2\right)$$
$$= \int Dq(\tau) \exp\left\{ -\frac{1}{\hbar} \int d\tau \left[\frac{m\dot{q}^2(\tau)}{2} + U(q(\tau)) \right] \right\}.$$

Thirdly, the obtained expression should be calculated in the limit $p \to \infty$ using multidimensional method of steepest descent. Wherein the main role is played by the analytical structure of the integrand, determined by the form of the potential $U(q)$. For example, when $k > 0$, $0 < \alpha < 2$, the asymptotics of the momentum distribution function is the Maxwell distribution multiplied by p in a positive degree depending on α.

Properties and dynamics of nanosecond laser-induced microplasma under spatial confinement

Samokhvalov A A[@], Veiko V P and Volkov S A

ITMO University, Kronvergskiy 49, Saint-Petersburg 197101, Russia

[@] samokhvalov.itmo@gmail.com

The properties and dynamics of laser-induced microplasma (LIMP) under conditions of spatial confinement are very different compared to its free expansion. Under such conditions, the plasma particle density and recombination rates can increase significantly. These factors leads to the fact that LIMP can effectively affect a transparent media which limits its expansion. In this work, plasma induced by laser ablation of a graphite target contacting with a transparent solid medium (fused silica) was studied. Here, we investigated the dynamics of LIMP and its main parameters. The thresholds and lifetimes of carbon radicals (Swan bands), silicon atoms and ions in LIMP emission spectrum were studied. The appearance of silicon lines (Si I) corresponds to the formation of a second plasma front in a fused silica. Using the LIMP continuum radiation, the electron temperature was calculated. Stark broadening of the silicon line (Si I 288.16 nm) was used to calculate of electron density. LIMP single ablation craters in fused silica were studied by white-light interferometry. In our opinion, the main application of such LIMP is precision micromachining of transparent dielectrics. The reported studies is funded by the Government of the Russian Federation (grant No. 074-U01) for the ITMO University.

Kinetic surface effects of laser nanoplasma

Bystryi R G[1,2]

[1] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

broman.meld@gmail.com

Plasma resulting from the interaction of laser radiation and nano-objects is a new and poorly studied object [1]. We will call such a plasma a nanoplasma. The results of the experiments caused interest in it. It has been shown that nanoplasma is a promising source of charged particles and radiation [2]. The experiments demonstrated the high efficiency of pumping laser energy into the energy of emitted particles or the energy of soft x-ray radiation. However, it turned out that the construction of quantitative models is tough. Some phenomena, such as the two-temperature electron emission spectrum, are inexplicable even qualitatively [3].

In this work, molecular dynamics modeling of surface phenomena occurring in a nanoplasma is presented. Spill out of electrons and the thermal emission of electrons are considered. A phenomenological theory of the observed phenomena is suggested. It was shown that some of them could not be described earlier, because they go beyond the boundaries of hydrodynamic models [4]. They can only be described by considering the kinetics of individual particles.

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Non-adiabatic effects and exciton-like states during insulator-to-metal transition in warm dense hydrogen

Fedorov I D[1,2,@]**, Orekhov N D**[2,1] **and Stegailov V V**[2,1,3]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[3] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

[@] ilya.d.fedorov@phystech.edu

The insulator-to-metal transition in warm dense hydrogen is one of the unresolved problems of recent decades. There are a large number of experiments aimed at determining this transition, but they have a large number of disagreements. One of the most used theoretical methods is the Born–Oppenheimer dynamic with finite-temperature density functional theory. This method assumes that at each step the system has a certain average (fractional) distribution of electrons over states. Accordingly, it is important to understand that for this method to work, it is necessary that the electron transition times between these states are significantly less than the molecular dynamics step. We analyze the dynamics of this transition and show its non-equilibrium non-adiabatic character overlooked in both interpreting experimental data and in theoretical models. The non-adiabatic mechanism explains the strong isotopic effect [1] and the large latent heat [2] reported recently. We demonstrate the possibility of formation of intermediate exciton-like molecular states at heating of molecular hydrogen, which can explain puzzling reflectivity and conductivity data at the insulator-to-metal transition [3].

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Unified data set for transport and radiation properties of noble gases

Deminsky M A[1,2,@]**, Petrunina E M**[1,2]**, Vasilievsky S A**[3] **and Potapkin B V**[2]

[1] National Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia
[2] Kintech Lab Limited, 3rd Khoroshevskaya Street 12, Moscow 123298, Russia
[3] Institute for Problems in Mechanics of the Russian Academy of Sciences, Vernadskogo 101-1, Moscow 119526, Russia

[@] de_minsky_m@kintechlab.com

This paper presents a methodology and a detailed set of data upon the transport and radiation properties of noble gases (He, Ne, Ar, Kr, Xe) and their mixtures in a wide temperature range ($T = 0.3$–50 kK) and pressure ($P = 0.1$–300 bar) under the assumption of local thermal equilibrium. Transport coefficients were calculated in the framework of Chapman–Enskog theory in the second approximation. Effective thermal conductivity was calculated as a sum of translational thermal conductivity and reactive one, which was obtained from the advanced version of Butler–Brokaw formula. For calculating collision integrals, the most recent theoretical and experimental data on the scattering cross-sections and interaction potentials was used. The comparison of different approaches for calculating collision integrals is also presented. Absorption coefficients were calculated based on data set of electronic energy levels, transition probabilities of atoms, potential energy curves and transition dipole moments of excimers. The generalized approach for bound-bound transitions together with Kramers–Unsold–Biberman model for photoionization were used for atoms. The characteristics of probabilities for unknown or not well-defined transitions between high excited states were calculated by method of quantum defect using quasiclassical approach for wave functions. Doppler, quasistatic, impact, Stark, van der Waals broadening mechanisms were taken into account for line shape. A numerical realization of described above approaches was implemented in the Fluid Workbench program suit.

The Moon surface latitude and dusty plasma

Dolnikov G G[@], Zakharov A V, Kartasheva A A, Bychkova A S, Shashkova I A, Kuznetsov I A, Lyash A N and Popel S I

Space Research Institute of the Russian Academy of Sciences, Profsoyuznaya 84/32, Moscow 117997, Russia

[@] dolnikov@mail.ru

The lunar exosphere is regularly exposed to solar wind and ultraviolet radiation. The investigation atmosphereless formed dusty plasma is existed the scientific instrument PmL that is intended both for the direct detection of the flux dust particles over the surface of the Moon and for the measurements electric field. Onboard descent modules in nearby Russian Luna space mission the instrument PmL have a chance to measure the lunar dusty plasma environment and electric field. The features of future missions are the landing place nearby Boguslavsky crater (70° south latitude). The consideration of calculations is showed the dependence of the surface potential, the Debye radius and electrical field from landing place on the Moon.

Dusty plasmas at the Moon: Effects of magnetic fields

Izvekova Yu N[1], Kassem A I[2], Popel S I[1,@], Morozova T I[1] and Zelenyi L M[1]

[1] Space Research Institute of the Russian Academy of Sciences, Profsoyuznaya 84/32, Moscow 117997, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] popel@iki.rssi.ru

The processes associated with the presence of magnetic fields, which may be important in a dusty plasma on the Moon, are considered. Lower-hybrid wave processes under interaction of the Earth's magnetotail with dusty plasma near the Moon's surface are described. Lower-hybrid waves are excited due to the relative motion of magnetospheric ions and charged dust grains that results in establishing the well-developed lower-hybrid plasma turbulence. The effective collision frequency characterizing the anomalous loss of ion momentum due to ion-wave interaction, as well as the electric fields arising in the system are found. It is shown that the electric fields excited due to the development of lower-hybrid turbulence are somewhat weaker than those arising due to the charging of the lunar surface under the action of solar radiation. Nevertheless, they are quite significant to affect the electric field pattern above the Moon. The obtained effective collision frequencies should be taken into account when deriving hydrodynamic equations for dusty plasma ions with allowance for their turbulent heating. Problems related to the consideration of magnetic fields, which can be important for detailed study of the dusty plasmas at the Moon, are stated. The possibility of generation of wave motions in the near-surface lunar plasma should be taken into consideration when interpreting the observational data.

Electrophonic noises from meteors and dust acoustic modulational perturbations

Morozova T I[@] and Popel S I

Space Research Institute of the Russian Academy of Sciences, Profsoyuznaya 84/32, Moscow 117997, Russia

[@] timoroz@yandex.ru

The present paper discusses dusty plasmas processes in the Earth's ionosphere associated with the passages of meteoroids and the spread of the meteor tail. Mechanisms explaining the occurrence of electrophonic noises recorded simultaneously with the passage of meteor bodies are suggested for extremely low frequencies range. It is explained by modulationalal instability of electromagnetic waves from meteor associated with the dust acoustic mode with characteristic frequencies 0.03–60 Hz. As electromagnetic waves propagate in the dusty plasmas of the meteor tail or in the dusty ionospheric plasmas, dust acoustic waves are excited as a result of the development of modulationalal instability of electromagnetic waves at characteristic frequencies and as a result, the electromagnetic waves become modulated. At the surface, these perturbations can be converted into sound waves by means of receivers. The growth rates of modulational instability at which the modulational excitation of extremely low-frequency dust acoustic disturbances occur are calculated. The conditions of the development of modulational instability are given. The correlation between observations of ionospheric radio noises and passages of meteors is noticed. Observed data of electrophonic noises include discussing range of frequencies 0.03–60 Hz.

Dust cluster rotation in a stratified dc discharge under action of strong axial magnetic field up to 2.2 T

Dyachkov L G[1,@]**, Dzlieva E S**[2]**, Novikov L A**[2]**, Pavlov S I**[2] **and Karasev V Yu**[2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Saint-Petersburg State University, Universitetskaya Naberezhnaya 7/9, Saint-Petersburg 199034, Russia

[@] dyachk@mail.ru

An experimental study of the influence of strong magnetic fields on dust structures in a stratified glow discharge is ongoing at Saint-Petersburg State University. To date, the rotation of dust clusters in magnetic fields B up to 2.2 T has been investigated. It was previously shown that after rotation inversion, the vectors of the angular velocity Ω and the magnetic field B coincide in direction. Inversion occurs at $B \approx 0.02$–0.05 T, and then the velocity Ω grows with increasing B almost linearly. In this case, the entrainment of dust particles by a rotating gas under the action of eddy currents arising in the striations becomes the main mechanism of rotation. In this experiment, we have shown that in fields $B \sim 1$ T, the rotation velocity ceases to grow and remains at the level of several rad/s. To explain this, we took into account factors that were not previously taken into account when describing the rotation of dust clusters: friction between gas layers rotating at different velocities in the striation and even in different directions; an increase in the length of striations in magnetic fields; plasma parameter oscillations inside the stratum. As a result, we have obtained satisfactory agreement between the theory and experimental data.

Reasons for rotating of dust structure in a highly non-uniform magnetic field

Dzlieva E S[@], Karasev V Yu, Pavlov S I and Novikov L A

Saint-Petersburg State University, Universitetskaya Naberezhnaya 7/9,
Saint-Petersburg 199034, Russia

[@] plasmadust@ya.ru

The problem of the investigation of the volume dust structures in the glow discharge strata in the strong magnetic field is the disruption of the stability of the dust trap as the magnetic field increases. In our experiments carried out in cryomagnet it was found that near the upper end of the solenoid in the strong magnetic field a stable dust trap is formed. The dust structure here rotates with an angular velocity of up to 10 rad/s in a direction opposite to the magnetic induction vector. Possible causes of rotation and quantification are discussed in this paper. First, this is the ion drag force in strata at radial ion flow in the longitudinal magnetic field. Second, this is the dragging by the rotating gas in striation. This mechanism causes the rotation of another sign then the observed one. Third, it is possible to consider the gradient drift of plasma (primarily ions) in a non-uniform magnetic field. But, according to the measurements made, the radial gradient of the longitudinal component of the field is extremely small. A feature of the dust trap being studied is the highly non-uniform magnetic field in which the discharge current channel expands and its radial component appears. The Ampere force here is possible because of the radial component of the current and the longitudinal component of the magnetic field.

Creation of stable plasma-dust structures in the striation of a glow discharge in the magnetic field

Pavlov S I[@], Dzlieva E S, Karasev V Yu and Novikov L A

Saint-Petersburg State University, Universitetskaya Naberezhnaya 7/9,
Saint-Petersburg 199034, Russia

[@] s.i.pavlov@spbu.ru

Recently, many works have been published upon the study of dusty plasmas produced both in a glow discharge and in a high-frequency discharge in a magnetic field. In studies of dusty plasma in glow discharge striations in a magnetic field, experimenters were not able to create stable dust structures in a magnetic field of more than 1000 G. This is due to various factors, one of which is the current-convective instability of a stratified discharge in a magnetic field.

This work is devoted to the description of an experiment to create a stable dust formation in a stratum of a glow discharge in a magnetic field up to 15 000 G. The dependence of the angular velocity of rotation of the structure on the induction of the magnetic field is obtained. Under observation, a magnetic field range was found in which current-convective instability is appear—partial degradation of the dust structure occurs.

Diagnostics of dust trap by the discharge glow in magnetic field

Novikov L A[@], Karasev V Yu, Dzlieva E S and Pavlov S I

Saint-Petersburg State University, Universitetskaya Naberezhnaya 7/9,
Saint-Petersburg 199034, Russia

[@] leontiy.novikov@gmail.com

In our previous works on the dynamics of dust structures in strata in strong magnetic fields, it was not technically possible to visually monitor the change of strata configuration. For the full understanding of the processes in stratified discharge in the magnetic field we carried out a new experiment where this was possible. In the experiment the video recording of stratified discharge in the longitudinal magnetic field at magnetic induction values from 0 to 2700 G was carried out. As the magnetic field increased, both the configuration of the strata and the intensity of their glow changed. The conditions of the experiment were chosen the same as in previous works. A magnetic coil was used to create the magnetic field, creating a field of up to 2700 G. Video recording was made by a periscope video camera with the possibility of displaying an image on a computer. The obtained results were compared with literary data.

Electrostatic interaction of dust particles with nonuniform surface charge distribution

Filippov A V[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia

fav@triniti.ru

The Janus or spotted particles, which are particles with two different hemispheres or regions on the surface, have recently attracted increasing attention in physics, biology, materials science, etc because of their asymmetric surface properties [1, 2]. To solve the problem of the electrostatic interaction of such particles, it is necessary to consider the nonuniform distribution of the free charges on their surfaces. A similar problem arises when considering nanoscale particles that carry only one or several elementary charges [3] and the assumption of a uniform distribution of free charge is a poor approximation. In this work, we solve the problem of the interaction of particles with an inhomogeneous distribution of the free surface charge in the form of δ-functions of angular variables. The dependence of the interaction force on the interparticle distance is determined for different values of the dielectric permittivity of the particles. Methods have been developed for regularizing the sum of poorly converging series in determining the total charge surface distribution.

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Spherical finite size particles interaction in equilibrium plasma

Pautov A A[1,2,3,@]**, Filippov A V**[1,2] **and Rodin M M**[1,2,3]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia
[3] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] pautov@phystech.edu

The interaction potential is important in many processes in a complex plasma or electrolyte, for example, for the formation of ordered or chain structures, the formation and attention of acoustic dust waves, coagulation and agglomeration of dust particles, etc. In this case, it is necessary to take into account the effect of plasma screening of the electrostatic interaction of charged dust particles. In [1], such an account was performed within the framework of the linearized Poisson–Boltzmann model. In the process of solving the problem, the MacDonald addition formula was used, which contains the Gegenbauer polynomials and the resulting series for determining the coefficients of the system of algebraic equations that determine the coefficients of the expansion of the potential in Legendre polynomials included double sums. In this work, we used a different addition formula leading to a single sum, which greatly simplifies the determination of the force and potential of the electrostatic interaction of dust particles and, accordingly, the coagulation rate constants of dust particles. This work is supported by the Russian Science Foundation (project No. 16-12-10424).

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Phase coexistence in Yukawa systems by the Kofke integration and a two phase approach

Reshetniak V V[1,@], Reshetniak O B[1] and Filippov A V[1,2]

[1] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] viktor.reshetnyak84@gmail.com

The conditions of phase equilibrium were studied for the bcc crystal and Yukawa liquid by molecular dynamics simulation. Calculations performed by two different approaches, supposing investigation of single-phase and two-phase systems near the melting line. In the first approach the melting line was determined using the Kofke integration algorithm [1]. The second approach is based on study of the stabilization at constant volume and energy of a two-phase system, which initially was slightly shifted from the equilibrium. Herewith the phase boundaries initially were specified flat. The methods don't use assumptions of [2], related to the solution of linearized equations of phase equilibrium.

The values of the commonly used melting and crystallization criteria were estimated. Results show that the change of the criteria along the melting line is less than 10%.

Special attention is paid to the study of the melting line at different values of the parameters of the interaction potential. As melting and crystallization lead to an abrupt change in density, the self-similar solution of the equations of motion cannot be obtained. Thus, calculation of the melting line with the use of the couple of the dimensionless parameters contains an uncertainty. Nevertheless, results of this paper show that this uncertainty is less than 3% in the selected range of parameters.

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Kinetics of crystallization of a supercooled Yukawa fluid

Reshetniak O B[1], Reshetniak V V[1,@] and Filippov A V[1,2]

[1] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] viktor.reshetnyak84@gmail.com

In the present work, the rates of formation and growth of the crystalline phase in the supercooled liquid of Yukawa were investigated numerically and analytically. The analytical model was based on the classical nucleation theory and used the parameters calculated by the method of molecular dynamics (MD): the specific energy of the phase boundary, γ, and the difference of the chemical potentials, $\Delta\mu = \mu_{\mathrm{bcc}} - \mu_{\mathrm{liq}}$. The value $\Delta\mu$ was calculated with the assumption of linear temperature dependence, using the results of [1]. The value of γ was calculated similarly to [2] for the (100) crystal surface. The obtained data were compared with the results of the direct MD simulation of crystal formation and growth in supercooled Yukawa fluid. The approach proposed by Sun [3], which based on the utilization of an external harmonic potential for a small part of the particles of the ensemble, was applied to accelerate the critical nucleus formation process. The simulations were performed for four different points along the melting line at a constant temperature of $T = 300$ K. The results show that the dimensionless specific energy of the phase boundary $\tilde{\gamma} = \gamma\delta^2/(k_B T)$ monotonically increases with the growth of the structural parameter, $\kappa = \delta/\lambda$. Here δ is the mean interparticle distance, λ is the screening length. The dependence of the crystal growth rate on κ, obtained directly in the MD simulations, qualitatively corresponds to the dependence of $\tilde{\gamma}(\kappa)$.

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Electrostatic interaction between two charged macroparticles in the presence of third point-like particle

Rodin M M[1,2,3,@] **and Filippov A V**[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia
[3] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] mrodin@triniti.ru

The issue of electrostatic interaction between charged bodies arises in the study of dusty plasma and electrolytes, molecular clusters, and extraterrestrial atmospheres [1]. A possible approach to model such systems is to consider a pair of charged dielectric spheres. Under this paradigm, researchers explained the phenomenon of attraction between like-charged macroparticles, which is experimentally observed [2, 3]. In this work, we made the first step to take into account the effect of surrounding particles on the pair by adding a third macroparticle to the system. For simplicity, we assumed the third particle as point-like (i.e., non-polarizable) and examined how its position affects the repulsion-attraction transition between the two spheres. We also varied the parameters of the two-particle system to find the configurations for which the effect of the third particle is strongest. Results include data for the net interaction force and bound charge distribution on the surface of the macroparticles that causes the onset of attraction between the spheres.

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Experimental study of the nonreciprocal effective interactions between microparticles in a gas discharge

Sametov E A[1,2,@]**, Kononov E A**[1,2]**, Lisin E A**[1,2]**, Vaulina O S**[1,2]**, Vasiliev M M**[1,2] **and Petrov O F**[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 141701, Russia

[@] sametov@phystech.edu

In the present work, we experimentally study how the symmetry of the interaction between microparticles in a plasma medium is broken. The "violation" of the interaction symmetry may be intrinsic for open and nonequilibrium soft matter of different nature, including catalytically active colloidal suspensions and complex (dusty) plasmas, where the geometry of interactions between particles plays a key role in the processes of self-organization, self-assembly, transfer and redistribution of energy.

For analysis of experimental data obtained in a dc gas discharge we developed a unique experimental method based on an analysis of the spectral density of random processes in an open dissipative two-particle system. To the best of our knowledge, this is the first detailed study of the nonreciprocal interparticle interaction forces that act between microparticles in a dc gas discharge

The results open novel prospects of investigations of various problems in physics of disperse systems with broken interaction symmetry, where the dynamical and structural characteristics of the system depend on the geometry of interactions between particles.

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Dynamics of active Brownian particles in a gas discharge plasma

Arkar K, Vasiliev M M[@] and Petrov O F

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

[@] mixxy@mail.ru

Active Brownian movement is widespread in nature, observed in the Earth's atmosphere, in biological and colloidal solutions, in plasma with a condensed dispersed phase, as well as in financial models [1]. In contrast to passive Brownian particles, active particles, also known as self-propelled Brownian particles or micro- and nano-swimmers, are able to absorb energy from the environment and transform it into directional movement. Active particles can be both biological and artificial objects [2]. For example, motile cells and bacteria or artificial micro-swimmers [1, 2].

In our work, we present the results of an experimental study of the behavior of a solitary dust particle in an electrostatic trap in plasma of a high-frequency capacitive low pressure discharge under effect of laser radiation with different power output. Within the framework we studied the dynamics of microparticles with various surface properties, including: non-absorbing laser radiation melamine formaldehyde (MF) particles; copper-coated MF laser absorbing particles; and Janus particles. Depending on the type of surface of the particles, their active Brownian motion was established. The trajectories, linear displacements, mean square displacements, and kinetic energies of dust particles were obtained depending on the driven laser radiation.

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Self-exited dust-acoustic waves in weakly coupled dusty plasma

Alekseevskaya A A[1,2]**, Trukhachev F M**[1,2,3,@]**,
Boltnev R E**[1,2]**, Vasiliev M M**[1,2] **and Petrov O F**[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 141701, Russia
[3] State Institution of Higher Professional Education "Belarusian–Russian University", Mira Avenue 43, Mogilev, Minsk Region 212000, Belarus

[@] ftru@mail.ru

The main feature of dusty plasma is its non-ideality described by the Γ parameter—the ratio of the potential energy of the interaction of dust particles to their average kinetic energy. At large Γ, a dusty plasma crystal is formed at an elevated pressure of a neutral gas. In this case, the dissipation of the kinetic energy of dust particles increases, which leads to an increase in the Γ parameter. Waves in such a plasma are described in [1]. Also, waves were observed in a monolayer of a strongly coupled dusty plasma in an rf discharge [2]. With a decrease in pressure, Γ decreases to 1–10 and the dusty plasma passes into the "liquid" phase. Dust-acoustic waves in the "liquid" phase were reported in [3,4]. However, waves in the "gas" phase, at $\Gamma < 1$, were not previously reported. At the same time, dust-acoustic waves in the gas phase are the best model of ion-acoustic and electron-acoustic waves. We, for the first time, carried out an experiment to study dust-acoustic waves in weakly coupled glow discharge plasma ($\Gamma < 1$) at the cryogenic temperature of the buffer gas. The main parameters of plasma and waves are measured.

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Structural phase transition in chain structures of active Brownian particles

Kononov E A[1,2,@]**, Vasiliev M M**[1,2] **and Petrov O F**[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 141701, Russia

[@] GADvin@yandex.ru

This work is devoted to the experimental study of structural phase transitions in chains of active particles. Change of the localization of active copper particles and structural phase transition in a cluster of chain structures with power increase of the heating laser radiation was observed. The analysis of the trajectories, dynamic entropy, and mean square displacement of the particles in the cluster reflects a change in the dynamics of particle motion with increasing laser radiation power: at values of laser radiation power less than 225 mW, the chain structures were stable, and the particles within chains moved slowly while being confined; at values of laser radiation power from 225 to 380 mW, the particles left their potential wells and began to move inside the shells of chain structures; with a further increase in the power of the acting laser radiation to 980 mW, the chains began to "exchange" particles. Thus, the dynamics of particle motion in a cluster of chain structures changes depending on magnitude of laser radiation power and corresponds to three modes: motion in a potential well, Brownian motion and combined directional chaotic motion consisting of laser-induced (photophoresis) and Brownian motion. An analysis of the linear displacement along and across the direction of motion of the particles at different values of the laser radiation power showed that a change in the dynamics of particle motion and a structural phase transition with the exchange of chain fragments inside the cluster became possible due to the mechanism of conversion of optical radiation energy into particle motion energy, i.e., due to the activity of copper particles.

Modeling the dynamics of macroparticles in a quasi-two-dimensional plasma–dust system under the influence of photophoretic force

Fairushin I I[@], Petrov O F and Vasiliev M M

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

[@] fairushin_ilnaz@mail.ru

In this paper, the Brownian dynamics technique is used to study the influence of the photophoretic force upon particles of a quasi-two-dimensional plasma–dust system for various values of the non-ideal system parameter and radiation power. It was found that the effect of laser radiation can lead to the appearance of the nature of particle motion inherent in the so-called active matter. In the work, the time dependences of the mean square and average linear particle displacements are calculated. It is established that when a photophoretic force acts on a colloidal dust system for the mean square displacement of particles in such a system, sections corresponding to ballistic, transition, and diffusion regimes are observed. Moreover, the average linear displacement for the particles is nonzero, which also characterizes them as active [1]. It also depends on the initial non-ideality parameter of the dust system and the power of the laser radiation acting on it.

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Collective particle dynamics in one-component Yukawa liquid: Self-consistent relaxation theory

Mokshin A V[@] and Fairushin I I

Kazan Federal University, Kremlyovskaya Street 18, Kazan, Tatarstan 420008, Russia

[@] anatolii.mokshin@mail.ru

A one-component plasma is the most suitable multiparticle system for the development of the microscopic theory of liquids. This is mainly due to the specific potential of interparticle interaction, as well as due to available experimental data and the results of molecular dynamics simulations, which can be used to verify the correctness of theoretical conclusions. In this work, we will present the microscopic theory of the collective dynamics of particles (ions) of a single-component plasma, where only the interaction potential—the Yukawa potential—and the structural characteristics—the particle pair distribution function and the structure factor—are used as input parameters. It will be shown that the microscopic theory is realized on a wide range of wave vectors; it generalizes the hydrodynamic theory and reproduces the known hydrodynamic expressions in the long-wavelength limit. The theory correctly reproduces all the known features of the spectra of the dynamic structure factor for a wide range of wave numbers, as well as the dispersion law of acoustic-like collective excitations. The theoretical results obtained are compared with the results of known theoretical models and approaches. This work was supported by the Russian Foundation for Basic Research (project No. 18-02-00407).

Non-linear screening effect in thermodynamics of asymmetric complex 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 141701, Russia

[@] martina1204@yandex.ru

The so-called "Debye–Hückel plus hole" approximation [1] was modified when the non-linear screening effect is taken into account in a highly asymmetric complex plasma of macroions and microions. Parameters of the non-linear screening of the macroions were obtained within the framework of the Poisson–Boltzmann approximation [2]. Two effects are found as a result of such calculations: (i) subdivision of all microions into two subclasses, bound and free ones, and (ii) significant reduction of an effective charge Z^* of the macroion in comparison with its true value Z due to the appearance of a thin high-density envelope of the bound microions around the macroions. The value of Coulomb interaction energy differs considerably in the case when the non-linear screening is taken into account. Microions correlations are considered in the present work.

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On the applicability of the persistence length for the analysis of the particle dynamics in a strongly coupled active matter

Lisin E 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 141701, Russia

eaLisin@yandex.ru

Active matter systems are able to take energy from their environment and drive themselves. It is well known that, on average, an individual active Brownian particle in a homogeneous environment will move along the direction of its initial orientation for a finite persistence length before its direction is randomized.

Redistribution of stochastic kinetic energy in two-dimensional ensembles with non-identical charged particles

Kaufman S V[1,@] **and Vaulina O S**[2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] wolf.reborn@mail.ru

The processes of energy exchange in systems of unequal interacting particles (that is, particles of different sizes, charges, etc) with a spatially inhomogeneous distribution of stochastic sources of kinetic energy are considered.

In a complex (dusty) plasma, the sources of the non-uniform distribution of stochastic kinetic energy for charged dust particles are inhomogeneous buffer plasma parameters in external electric fields and changes in the charges of dust particles caused by the random nature of ion and electron currents charging these particles. Sources of uneven heating of the dust particle system can also be inhomogeneous temperature distribution of the surrounding gas, laser radiation used for diagnostics, etc.

Theoretical model for analysis of energetic balance in such systems was considered. Based on this model, analytical relations, describing redistribution of stochastic kinetic energy between interacting particles in the system, were obtained. Proposed relations were checked by numerical simulation of a problem for systems of two particles with Coulomb interaction. The numerical and theoretical analysis of the processes of energy redistribution in extended two-dimensional ensembles of non-identical particles consisting of two different fractions, taking into account the forces of ion entrainment, is performed.

Results of this paper can be applied for systems with any type of reciprocal interaction and can be useful for analysis of energetic exchange in inhomogeneous systems, which are of interest in physics of plasma, and in physics of polymers and colloidal systems.

Radial inversion of ion flows in a dense dust cloud in a dc discharge

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

[@] cryolab@ihed.ras.ru

The electrical characteristics of the positive glow discharge column with a diameter of 1.65 cm and the plasma parameters in pure neon and in plasma with different density of 2.55-μm dust particles were modeled using a diffusion-drift model [1]. It was found that the density of dust particles affects the direction of drift flow of ions in the dust cloud. At a low density of dust particles (with number density less than 1×10^{11} m^{-3}), the density of ions in the center of the dust cloud may be higher than that at the boundary, and then the drift flow of ions coincides in direction with the diffusion flow of ions. In this case, the both flows are directed towards the discharge tube walls. At a higher density of dust particles in a dust cloud the drift ion flow and the diffusion ion flow change direction to the center of the discharge. In this case, the drift and diffusion flows of ions inside the dust cloud do not coincide in direction with these flows outside the dust cloud in the discharge area free from dust particles. It was found that that the change in the direction of the drift ion flow is caused by inversion of the radial electric field inside the dust cloud. The inversion of the radial electric field was previously obtained for the first time for air [2]. The inversion of the radial field occurred as a result of strong depletion of the electron density profile inside the dust cloud. The redistribution of electrons caused a redistribution of ions and a change in the direction of ions diffusion.

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Termophoresis in neon dc discharge plasma with dense dust structures

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 thermophoresis phenomenon in a dc discharge in neon is studied in the presence of dense structures of charged dust particles. The experimental data on the formation of voids in dust structures formed by dust particles in a glow dc discharge in neon have been used. The simulation has been performed using the diffusion-drift model of the plasma of the positive column of a glow discharge in neon with microparticles [1] taking into account the heat release of the discharge. The dependence of the thermophoretic force acting on a charged dust particle on the density of the dust structure and gas pressure is analyzed. It has been shown that with decreasing gas pressure, the dependence of the thermophoretic force on the dust structure density increases due to the mutual screening of dust particles. An analogy was found between the dependence of the thermophoretic force in the plasma-dust structure on the distance between adjacent dust particles and its behavior near the wall bounding the plasma volume [2]. It has been obtained that as the gas pressure decreases, the dependence of the thermophoresis force on the concentration of dust particles increases due to their mutual screening. Comparison of these results with the data in different plasma-dust systems can provide a key to understanding the processes of heat and momentum transfer in gas media and plasma with condensed disperse phase.

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Solitary density waves in the one component Coulomb particle structures as experimental support of the general versatility of the caustic theory

Deputatova L V[@], Filinov V S, Pecherkin V Ya, Syrovatka R A, 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

[@] dlv@ihed.ras.ru

In the present work, it is shown that the generation of a solitary density wave in a strongly coupled single-component Coulomb system of particles enclosed in a long quadrupole electrodynamic trap of the Floor is possible when energy losses due to air viscosity can compensate for the contribution of the energy of the changing electric fields of the trap. Results of this paper allow to identify observed solitary waves as the caustics (according to definition by V I Arnold in the book "Catastrophe Theory") and can be considered as the new experimental support of the general versatility of the caustic theory in describing different physical phenomena not only in collisionless systems of particles but also when interparticle interaction and interaction with external fields in viscous media are strong.

Spatial separation of particles in an electrodynamic trap

Vladimirov V I[@], Deputatova L V, Filinov V S, Pecherkin V Ya, Syrovatka R A and Vasilyak L M

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

[@] vld@ihed.ras.ru

Numerical simulation and experimental studies of the spatial separation of the micron-sized particles have been done for a linear quadrupole electrodynamic trap. Numerical simulations were carried out for mixtures of two and three particle spices of different size and masses. Spatial separation was experimentally obtained for a polydisperse Al_2O_3 micron-sized particles of 10–40 μm. In numerical simulations, spatial separation was obtained both for different particle masses and charges provided the same ratio of the particle charge to mass. Calculations for experimentally observed charges of particles in a corona discharge were performed.

New method for cleaning air and dusty surfaces using variable electric fields

Syrovatka R A[@], Deputatova L V, Filinov V 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 work is aimed at solving the urgent problem of developing new methods for cleaning air and dielectric surfaces from dust particles. The problem of dust cleaning arises, for example, at nuclear and solar power facilities, in space missions. A promising cleaning method is the capture and non-contact removal of dust particles using variable electric fields created by electrodynamic traps. In the course of the work, a new method of air filtration and cleaning of dielectric surfaces from dust based on the capture and non-contact removal of dust particles by means of electrodynamic traps has been developed. The researches were carried out by methods of mathematical modeling and natural experiment.

Impact of charged particles on a strong shock wave in a weakly ionized gas: Numerical evaluation

Triaskin J V[@] and Pavlov V A

Saint-Petersburg State University, Universitetskaya Naberezhnaya 7/9, Saint-Petersburg 199034, Russia

[@] jaroslav.triaskin@spbu.ru

In this work, the interaction of strong shock wave (supersonic bodie) with low-ionized plasma is discussed. The basic principles of nonlinear ion-acoustic waves formation in a weakly ionized non-isothermal gas ($T_e \gg T_i \approx T_n$) subjected to a strong stationary shock wave of the neutral component is studied on the base of computer-aided calculations and analytical methods. The ion-acoustic approximation is employed to describe the plasma component of charged gas. Within a such approach the ion-acoustic waves arise via the collisions of charges with the neutral particles. The regularities found in the numerical analysis reveal an additional mechanism for reducing the intensity of a strong shock wave of the neutral component without the release of thermal energy in the region in front of the front. The reciprocal action of the charged components on the neutral particles lead to significant modification of the structure and reduction of the intensity of the shock wave. It was found that a weakly ionized plasma (unperturbed state) strongly affects the neutral component and reduces the intensity of the shock wave [1, 2].

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Thrust of synthetic jet and power characteristics of plasma actuators with various configurations at reduced pressure

Trifanov I V[1,2,@]**, Serebriakov D G**[1,2]**, Bocharnikov V M**[1] **and Golub 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 141701, Russia

[@] trifanovpgt@gmail.com

Symmetric actuators with various configurations creating a dielectric barrier discharge (DBD) can be used to control the lift force of the wing [1]. Under the influence of strong electric field a surrounding air is ionizing and accelerating. This leads to the formation of the synthetic jet, directed perpendicular to the surface of the wing in a given area. For a greater effect of the impact of synthetic jet on the flow the thrust must be greater with less energy coupling.

In the first half of this work, the dependence of the linear thrust and the specific thrust on the power of synthetic jets created by a symmetrical drive with various configurations on the air pressure corresponding to a flight altitude of up to 20 km was studied. At certain pressures, there are maxima in the dependencies.

In the second half of this work, the influence of the actuators on the flow and lift of the wing profile in the oncoming flow with different arrangement of actuators on the wing was investigated. In these experiments, the location of actuators on the wing and the thrust of the synthetic jet were varied. The lift was measured and shadow photographs of the flows near the wing were taken.

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About the efficiency of dielectric barrier discharge

Serebriakov D G[1,2,@]**, Trifanov I V**[1,2]**, Bocharnikov V M**[1] **and Golub 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 141701, Russia

[@] denser96@yandex.ru

For controlling the flow around the wings of an airplane, a dielectric barrier discharge (DBD) created by a plasma drive can be used [1]. The flight speed should be no more than 25 m/s; the Reynolds number Re $\sim 10^4$. Such conditions are achievable when flying unmanned aerial vehicles at an altitude of about 20 km. As the height increases, the pressure and temperature of the ambient air changes. Therefore the characteristics and properties of the DBD are also changing. Most of the existing works have been carried out at atmospheric pressure [2,3]. Our scientific group obtained the dependences of the dissipation coefficient of the source–actuator– DBD system, and discharge efficiency for a symmetric actuator with different lengths of external electrodes in previous papers and the results have shown that with decreasing pressure, the discharge efficiency increases significantly. In this paper, we investigated the electrical characteristics of DBD under reduced pressure for actuators various shapes (round, with a "floating" electrode, etc). It was shown that the ratio of the active component of power, which is determined by the efficiency of DBD, to the passive component of power, which is determined by the energy reserved in the actuator, is independent of pressure.

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Structure perturbations features created by a pulsed arc discharge in a boundary layer

Kazanskii P N[@], Moralev I A, Kotvitskii A Ya 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

In question of intensifying the mixing of the boundary layer one of promising methods is a pulse-periodic arc discharge in a magnetic field [1]. This paper presents an analysis of the structural features of the generated disturbances when the arc moves across the incident flow. Visualization of the flow is done by the PIV (particle image velocimetry) method. It showed that a vortex structure of 3–10 mm in size is formed. Its size and structure depend on the pulse duration (from 40 to 380 μs) and the current strength (from 30 to 80 A) of the discharge. In this case, the vortex thread closes to the wall with a short jumper in front of the perturbation, and gradually moves away from the wall at the upstream end. Kinematic transport in a vortex leads to a modification of the longitudinal velocity field. It can be seen that in the region where the vortex exists, a pair of regions with a deficit and an excess of velocity is formed, which correspond to the regions of downward and upward flow in the vortex.

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Formation and development features of the current channel in the long atmospheric discharge

Medvedev M A[1,2], Parkevich E V[1,2] and Oginov A V[1,@]

[1] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] oginov@lebedev.ru

Atmospheric discharges have a complex branched structure of current channels. In studies of spark discharges in air, it was discovered that current channels could be formed with microstructure, which represents a bunch plasma filaments. Those plasma filaments have extremely high ionization with electron density n_e up to $\sim 10^{20}$ cm^{-3} [1].

In this work, we presenting the experimental data on formation and development of the atmospheric discharge channel in the long gap (≈ 60 cm) obtained by laser probing. The high voltage generator can generate electrical pulses with voltage magnitude up to 1.2 MV and current up to 10 kA (ERG setup [2,3]). It was show that the leader discharge has a microstructure in the current channel and a bunch of thin microchannels at the channel tip. That microstructure is not clearly visible in the lightning-like stage of the discharge. But the current channel has another internal structure that represents the dense internal channel with longitudinal inhomogeneities.

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Research and localization of microwave sources of high-voltage laboratory atmospheric discharge using ultra-wide-band antennas

Baidin I S

Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

ibaydin@yandex.ru

The processes occurring in the initial phase of high-current pulsed atmospheric discharges that lead to the generation of radio radiation have been studied for a long time. For example, radio frequency radiation from lightning at frequencies over 500 MHz was first recorded by Takagi and Takeuchi in 1963 [1]. In the laboratory, this problem is still being investigated today. In [2], the authors were able to register radio pulses with a frequency of 2.4 GHz. But at this point, no one has been able to accurately study and locate the source of these radiations. In this work we presenting the experimental data on the localization of a microwave radiation source with frequencies of 1–4 GHz and in an atmospheric discharge channel in the long gap (60 cm). The high voltage generator can generate electrical pulses with voltage magnitude up to 1.2 MV and current up to 10 kA (ERG setup [3]). The results in the first approximation are consistent with experimental and analytical work on the research of lightning and laboratory spark discharges.

About the features of the fast explosive generation of anode spots in a nanosecond atmospheric discharge

Parkevich E V[@], Medvedev M A, Khirianova A I, Ivanenkov G V and Oginov A V

Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

[@] parkevich@phystech.edu

Here the formation of a millimeter-sized spark discharge in ambient air was studied on a nanosecond time scale using multi-frame laser interferometry, shadow, and schlieren imaging. The discharge was initiated in gaps formed by a point cathode and flat anode or vice-versa. It is found that the electrical breakdown of the gap is associated with an extremely fast ($\ll 1$ ns) explosive formation of micron-sized (≈ 10–50 μm) cathode and anode spots, whereas the characteristic delay between the instants of the anode and cathode spot initiation can be much shorter than 1 ns [1]. The spots appear as rapidly evolving near-electrode plasmas with an electron density $n_e \sim 10^{19}$ to 10^{20} cm^{-3}. The findings indicate that the extremely fast formation of anode spots is associated with an ultrafast gap breakdown promoted by an ultrafast ionization wave governed by the rapidly evolving cathode spot.

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Laser-triggered gas switch for precise electrophysical experiments

Medvedev M A[1,2,@]**, Parkevich E V**[1,2] **and Oginov A V**[1]

[1] Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] medvedevma@lebedev.ru

We present a practical air-filled switch triggered by a GW picosecond laser beam with slightly varying breakdown delay and low jitter. The switcher relies on the spark gap with a coaxial geometry, which is ignited by a focused laser beam directed at a certain angle to the gap axis. The switcher is integrated with a high-voltage cable generator operating at a constant negative voltage of up to 50 kV. We demonstrate that, by just varying the ignition angle of the spark gap, one can achieve a variable breakdown delay tunable within $\sim$ 0.1–10 ns with $\lesssim$ 1 ns jitter. Empirical dependences of switching characteristics of the developed device on the ignition angle are obtained. We demonstrate that, combined with variation of the ignition beam energy and charging voltage, variation of the spark gap ignition angle provides superior control over the gap switching characteristics without complicating the switch design. The proposed approach to driving the switching characteristics appears highly promising for designing compact Laser-Triggered Gas Switches with variable temporal characteristics and achieving precise synchronization between high-voltage and measuring equipment.

The simultaneous use of interferometry and schlieren photography in laser diagnostics of plasma objects

Khirianova A I[@], Parkevich E V and Medvedev M A

Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

[@] khirianova.alexandra@gmail.com

The paper investigates the task of increasing the accuracy of restoring information on the distribution of electron density of complexly structured plasma objects by processing the results of simultaneous interferometry and schlieren photography. Test modeling of schlieren and interferometric frames for objects of various geometries and density distributions was carried out. Interferogram modeling was carried out as a direct task based on solving a parabolic wave equation by the method of smooth perturbations [1]. The modeling of schlieren images was carried out in the framework of geometric optics approximations, based on the solution of the eikonal equation describing the trajectories of rays passing through an optical inhomogeneity. It is shown that the data extracted by schlieren photography in some cases significantly refines the results of processing interferograms.

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Air temperature spatial distribution in corona discharge with plane comb of metal rod electrodes obtained by schlieren technique

Pinchuk M E[1,@], Lazukin O M[2] and Stepanova O M[1]

[1] Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, Russia
[2] Timiryazev Institute of Plant Physiology of the Russian Academy of Sciences, Botanicheskaya 35, Moscow 127276, Russia

[@] pinchme@mail.ru

Air temperature spatial distributions in corona discharge with plane comb of metal rod electrodes are presented for negative and positive polarity determined by schlieren technique. This technique has very high sensitivity allowing measure a temperature difference in tenth centigrade at room temperature in gas flow. A absence of gas heating in the studied system was shown in the full range of the studied parameters.

Near electrode voltage drops in high-current high-pressure discharges with fast energy input

Bogomaz A A, Pinchuk M E$^{@}$, Budin A V and Leks A G

Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, Russia

$^{@}$ pinchme@mail.ru

Dependence of the total voltage drop near the electrode for high-current high-pressure discharges on the rate of rise of current in the discharge in the range from 10^9 to 10^{12} A/s at initial gas pressure of 10–200 MPa is presented. The proximity of the pressure values in the discharge channel to the magnetic pressure, significantly exceeding the initial gas pressures, allows to compare experimental data with a large difference at the initial pressures in the discharge system of such parameters with currents of 0.1–1.2 MA. A new technique for near electrode voltage drops determination is proposed at conditions of the fast energy input at $\mathrm{d}J/\mathrm{d}t = 6 \times 10^{11}$ A/s. The technique is based on measuring the characteristics of a shock wave detaching from the discharge channel. This data compared with data previous experimental researches for discharge in high pressure hydrogen [1–3]. Total near-electrode voltage drops were increased with in the current rise rate from around two hundreds to approximately ten thousand volts.

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[2] Savvateev A F, Budin A V, Rutberg P G, Bogomaz A A and Pinchuk M E 2004 *High Temp. Mater. Processes* **8** 617–25
[3] Bogomaz A A, Pinchuk M E, Budin A V, Leks A G, Leontev V V and Pozubenkov A A 2018 *J. Phys.: Conf. Ser.* **946** 012138

Average critical state model for explosive-electron emission plasma parameters estimation

Tsventoukh M M

Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

elley@list.ru

A complete model based on the transition through the critical state for explosive electron emission pulses in the cathode spot of a vacuum arc was developed by Mesyats and Tsventoukh [2015 *IEEE Trans. Plasma Sci.* **43** 3320] and Tsventoukh [2018 *Phys. Plasmas* **25** 053504]. This model predicts set of parameters for plasma of the cathode-spot explosive cells, in particular, average plasma density— about 10^{20} cm^{-3} the electron and ion drift velocity $\propto (T_{\mathrm{cr}}/M_i)^{0.5}$, explosive plasma momentum of tens of g cm/(s C), and the average ohmic electric field of few V/μm.

The relationship between the critical parameters of a surface material with a developed micro and nanostructure and the charge state of vacuum arc ions has been determined by Barengolts *et al* [2020 *Nucl. Fusion* **60** 044001]. It was proposed that reduction of effective critical temperature due to formation of nanostructure being responsible for the ion charge reduction.

The developed model is consistent with the latest experimental data from Zöhrer *et al* [2020 *Plasma Sources Sci. Technol.* **29** 025022]. Whereas the single-metal cathodes exhibit correlation in the plasma velocity and burning voltage with the corresponding critical temperatures the mixed materials demonstrate lower velocity and voltage that may be attributed to the their fine-stricture of surface.

The formation of shock waves during explosive processes at the cathode

Maiorov S A[1,@] **and Ragimkhanov G B**[2]

[1] Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova 38, Moscow 119991, Russia
[2] Dagestan State University, Magomeda Gadzhieva 43a, Makhachkala, Dagestan 367000, Russia

[@] mayorov_sa@mail.ru

The relevance of studying high-voltage nanosecond pulsed gas discharges is due to their wide practical application: plasma-stimulated combustion, plasma aerodynamics, plasma medicine, surface treatment. At the same time, the wide variety of physical processes occurring in them also determines the complexity of interpretation of observed phenomena. From a practical point of view, the study of spark discharges is of considerable interest, since they arise very often in high-voltage technology, including as a negative factor in the form of breakdown, leading to short circuits and having an erosive effect on electrodes and insulators. It is known that an expanding spark channel, acting as a piston, forms a cylindrical shock wave. In all cases, these waves propagate in a weakly ionized plasma. This work is devoted to the results of studies of the formation and propagation of shock waves from an expanding cathode spot and a spark channel, and the features of the formation of waves in magnetic fields. An explosive model of the development of the cathode spot involves the release of large energy at the emission center and subsequent heating and explosion of the micro-tip. It was shown that during a short time < 10 ns, an energy of 60 J/mg is released in the cathode spot. In this case, the cathode spot plasma is characterized by intense lines of ions of the cathode material and continuous radiation in a wide range of wavelengths (260–360 nm). The spectrum intensity was maximum in 20–30 ns.

High-enthalpy air high-voltage ac plasma torch

Subbotin D I[@], Surov A V, Popov V E, Popov S D, Kuchina Yu A, Obraztsov N V, Nikonov A V and Serba E O

Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, Russia

[@] subbotin1987@mail.ru

Plasma torches are used for welding, surface treatment, destruction of hazardous waste, processing of organic substances, etc. In most cases, such devices operate using direct current. Alternating-current plasma torches are used much less frequently. However, its have several advantages: high thermal efficiency, a relatively simple power source, the use of industrial current with a frequency of 50 Hz. This report examines a three-phase, high-voltage, ac plasma air burner. It consists of three channels of a water-cooled electric arc, each of which contains a copper rod electrode. The power of the plasma torch is regulated by the value of the electric current from the power source and the air flow. To stabilize the arc, a tangential vortex air flow is used. Initially, an electric arc is ignited between the plasma torch case and the rod electrode. Further, the air stream blows an electric arc to the nozzle of the plasma torch, where it is switched with the same arc from an adjacent channel. The power source of the plasma torch (10 kV, 50 Hz) consists of switching equipment, three current-limiting reactors, a reactive power compensator, measuring instruments and a step-up transformer (380/10 000 V). Due to the high inductance, this device is a current source (high degree of current harmonicity). Tests of the plasma torch were carried out at a current of 50 A. The power of the plasma torch was 61.7 kW with a minimum air flow of 5 g/s. The theoretical heat content of the plasma in this case was 12.34 MJ/kg. The obtained value significantly exceeds our previous results when working with air as a plasma-forming gas. In this case, peaks of re-ignition of the arc were not observed on the voltage oscillograms, which indicates the stable operation of the plasma torch.

Investigation of wood ash melting by ac plasma torch

Kirillova A A[1,@] and Subbotin D I[1,2]

[1] Saint-Petersburg State Technological Institute (Technical University), Moskovsky Avenue 26, Saint-Petersburg 190013, Russia
[2] Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, Russia

[@] feoctista-2016@yandex.ru

The accumulation of solid waste is a big environmental problem for humanity. There are several methods to process them: burning, gasification, smelting, etc. The most common method is burning, but during processing, ash is formed that contains a large amount of organochlorine compounds and heavy metals. Under the influence of water, these substances can get into the soil and pollute it. In this case, the most dangerous is fly ash, which has a low resistance to leaching. One of the methods for processing ash from waste incineration can be plasma treatment. In most cases, studies are carried out with inert gas systems. Sintered wood ash was melted in a lined reactor using an alternating current air plasma torch. The size of the processed pieces of sintered ash was 10–50 mm. The power of the plasma torch was 75 kW at an air flow rate of 8.8 g/s. Temperature control on the ash surface was carried out using a two-beam pyrometer. The total melting time was 7 h. The temperature of the least heated part of the melt was 1350 °C. A sample of molten ash was removed from the bottom of the reactor using a metal ladle (100 ml). Liquid slag was cooled in a large number of cold water. Upon contact of the hot molten slag with water, glass-like pieces 2–3 mm in size were formed. The composition and properties of the slag were studied using a scanning electron microscope with an attachment for elemental analysis and an x-ray diffractometer.

Synthesis of tungsten nanoparticles in high pressure abnormal glow discharge

Sofronitskiy A O[1,@], Fairushin I I[1,2,3] and Saifutdinov A I[1]

[1] Kazan National Research Technical University named after
A N Tupolev—KAI, Karl Marx Street 10, Kazan, Tatarstan 420111, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences,
Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[3] Kazan Federal University, Kremlyovskaya Street 18, Kazan, Tatarstan
420008, Russia

[@] artempic8@mail.ru

An experimental study of the synthesis of tungsten nanoparticles in a direct current discharge was carried out. The discharge mode corresponded to the anomalous glow discharge [1], argon was used as the plasma-forming gas, the cathode and anode were made of tungsten. The pressure ranged from 50–150 Torr, the voltage at the discharge was 300 V, the current strength varied from 300 to 650 mA. In the inter electrode region, a transverse argon flow was organized. The gas flow carried out from the discharge region the atoms and clusters of tungsten formed as a result of intense ionic bombardment of the cathode, from which nanoparticles subsequently formed. Next, the nanoparticles were deposited on a substrate. After the experiment, the surface of the substrate was investigated using a scanning electron microscope. On the surface, conglomerates of tungsten nanoparticles with a characteristic size of 5–50 nm were detected.

[1] Saifutdinov A I, Fairushin I I and Kashapov N F 2016 *JETP Lett.* **104** 180–5

Investigation of the transfer of isopropanol and water from the solution to the gas phase under the action of a dc discharge with a liquid cathode

Chistolinov A V[1,@], Yakushin R V[2], Perfilyeva A V[2] and Tyuftyaev A S[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Mendeleev University of Chemical Technology of Russia, Miusskaya Square 9, Moscow 125047, Russia

[@] a-chi@yandex.ru

In direct current (dc) discharges with a liquid cathode, nonequilibrium transfer of solvent molecules and dissolved substances to the gas phase occurs under the influence of ion bombardment of a liquid cathode, similar to the process of sputtering a cathode in a classical glow discharge. To characterize the transfer of a substance from a solution to the gas phase under the influence of a direct current discharge with a liquid cathode, a transfer coefficient is introduced—a value equal to the number of particles of this substance transferred unchanged from the solution to the gas phase per one ion bombarding the surface of the solution. We studied the dependence of the transfer coefficients of water and isopropanol on the distance between the electrode and the solution surface and the discharge current. The transfer is happening from the solution to the gas phase under the action of a dc discharge with a liquid cathode. It is shown that as the distance between the electrode and the solution surface increases, the water transfer coefficient increases, and the isopropanol transfer coefficient decreases. With the increase of discharge current both the transfer coefficients of water and isopropanol fall, and the transfer coefficient of isopropanol falls faster than the transfer coefficient of water. This work was partially supported by the Russian Foundation for Basic Research, grant No. 19-08-00592.

Investigation of the dynamics of filaments in a dc discharge with a liquid cathode

Yakushin R V[1], Chistolinov A V[2,@], Khromov M A[2] and Tyuftyaev A S[2]

[1] Mendeleev University of Chemical Technology of Russia, Miusskaya Square 9, Moscow 125047, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] a-chi@yandex.ru

It is known that near the surface of the liquid cathode, the discharge channel of the dc discharge with the liquid cathode is divided into separate filaments. In this paper, the dynamics of filaments in a dc discharge with a liquid cathode was studied using high-speed video recording methods. The study was conducted in the current range of 25–100 mA at different distances between the electrode and the liquid surface. High-speed video recording was performed with the Phantom VEO 410S color video camera, at a recording speed of up to 10 000 frames per second.

High-speed video recording showed that the filaments are in constant chaotic motion. Typical speeds are on the order of a few meters per second. The average number of filaments increases with increasing discharge current. Also, as the discharge current increases, the distance between the solution surface and the branching point of the discharge channel into filaments increases. At a certain critical current, the position of the branching point coincides with the electrode. At a current greater than the critical current, the discharge filamentation starts directly from the electrode. As shown by high-speed video recording, the number of filaments does not remain constant over time. The main mechanism for the formation of new filaments is the division of filaments. The main mechanism for the death of filaments is their movement to the periphery of the discharge and extinction in the characteristic time of hundreds microseconds.

Investigation of discharge plasma with a liquid cathode near the surface of a liquid cathode using emission spectroscopy

Chistolinov A V[1,@], Perfilyeva A V[2], Sargsyan M A[1] and Tyuftyaev A S[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Mendeleev University of Chemical Technology of Russia, Miusskaya Square 9, Moscow 125047, Russia

[@] a-chi@yandex.ru

In this paper, a dc discharge with a liquid cathode was studied using emission spectroscopy. As a liquid cathode, a solution of sodium hydroxide in deionized water was used. The discharge occurred at atmospheric pressure in the air. The image of the discharge was formed by a quartz lens on the plane in which the entrance hole of the spectrometer light guide was placed, which allowed the study of spectra in the selected discharge zone. The emission spectra of the discharge showed the presence of radiation bands of OH—radical, molecular nitrogen N_2, (2^+) and N_2, (1^+), molecular ion N_2^+ (the latter bands are very weak against the background of molecular nitrogen bands and are visible only near the liquid surface), as well as spectral lines of atomic hydrogen H I and oxygen O I. Experiments have shown that near the surface of the liquid, there is a sharp increase in the intensity of the atomic hydrogen lines H I. At a current $I = 100$ mA and an interelectrode distance of 2 mm, the rotational and vibrational temperatures of the plasma in the central part of the discharge near the liquid surface were determined using the emission spectrum of the second positive system of molecular nitrogen N_2, (2^+). They are $T_r = 2800$ K, $T_v = 3800$ K, respectively. This work was partially supported by the Russian Foundation for Basic Research, grant No. 20-08-00866.

The destruction of pure metal cathodes during the initiation of direct current arc

Sargsyan M A[@], Tereshonok D V, Gadzhiev M Kh, Tyuftyaev A S and Shcherbakov V V

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

[@] m.sargsyan86@mail.ru

In this research, the behavior of cathodes made from pure tungsten and pure hafnium in the direct current electric arc at 200 A and in atmospheric pressured argon medium was investigated. The research was focused on the processes happening with the cathodes during the arc initiation phase (first 100 ms after the power input). The processes of rapid cathode destruction were registered, and can be characterized as the destruction of the cathode in liquid phase due to electro-magnetic forces. Characteristic times of the whole process were recorded, as well as the changes in temperature fields on the cathodes surfaces and the rate of mass loss for both types of cathodes. It has been shown that the initial destruction of the cathode plays a major role in the cathodes resource life. These results may help in design of new plasma equipment especially in cases where the plasma should be kept clear of the cathode material, or in opposite cases where the cathodes material needs to be steadily added into the plasma stream.

Low-temperature plasma generator of nitrogen–propane mixture

Gadzhiev M Kh[@], Tyuftyaev A S, Kulikov Yu M, Sargsyan M A, Yusupov D I and Son E E

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

[@] makhach@mail.ru

One rather unconventional application of low-temperature plasma is the plasma gasification of domestic and industrial waste. This is considered a good application due to the fact that at a temperature of 4–5 kK, any substance is split into electrons, ions and radicals. The greatest thermal efficiency from the variety of low-temperature plasma generators is possessed by direct current plasmatrons, which have the highest stable mode and resource when using argon as a plasma-forming gas. When disposing of waste, the use of argon on an industrial scale is not economically feasible, therefore it is advantageous to use available gas mixtures, for example, nitrogen or air with the addition of a mixture of propane and butane. Because of this, a low-temperature plasma generator working on a mixture of nitrogen and propane was developed, with the possibility of supplying propane to the cathode region, to the arc burning zone, and also to the plasma stream below the arc binding zone. The maximum propane flow rate for a given plasmatron design and plasma-forming nitrogen flow rate, at which the arc stability is not disturbed, was determined. When propane is supplied into the arc binding zone, the decay products are deposited mainly on the electrodes, and when it is supplied to the anode after the arc binding spot, the decomposition products are deposited mainly at the anode exit. The study of the microstructure and analysis of the phase composition of the decomposition products of propane was performed.

On plasma thermal spraying by the torch with divergent output nozzle

Son E E[1], **Vetchinin S P**[2], **Gadzhiev M Kh**[2,@],
Yusupov D I[2], **Tyuftyaev A S**[2], **Chinnov V F**[2] **and
Sargsyan M A**[2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9,
Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences,
Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] makhach@mail.ru

The analysis of the current state of the technological process and
equipment for plasma thermal spraying and coating of various pow-
der materials has been carried out. To increase the processing effi-
ciency during the deposition of ceramic materials and refractory al-
loys a novel technological scheme of plasma spraying with a powder
feed axially to the cathode was proposed and preliminarily tested.
Basing the plasma torch with an expanding channel of the output
electrode its plasma-spraying version has been developed in which
the sprayed powder is supplied both to the cathode or anode arc
striking zone and to the current-free plasma jet. The electrophys-
ical parameters of the argon plasma torch and the speed, size and
temperature of particles of a sprayed powder were investigated. It
was shown that the particle velocity of Al_2O_3 powder depending on
the gas flow and arc current reaches up to 100 m/s. The tempera-
ture of the powder particles in the vicinity of substrate at a current
of 300 A is about 2400– 2500 K.

Atmospheric-pressure electrode microwave discharge at continuous and pulse-periodic magnetron generation modes

Chepelev V M[1],[@], Antipov S N[2] and Gadzhiev M Kh[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Limited Company "AGNI-K", Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] chepelev@ihed.ras.ru

The prototype 2.45 GHz multipurpose plasmatron, which was developed and manufactured earlier, allows the generation of cold atmospheric pressure plasma jets using an external portable discharge chamber (plasma torch) with a wide output with a diameter of 2.5 cm and a power of mW up to several hundred watts. Discharge channels are formed in argon flow between the rod-like electrodes and the inner wall of the discharge chamber near the outlet of the chamber. We studied the temporal features of the formation of a microwave discharge in the torch in continuous and pulse-periodic modes of magnetron power supply. For the plasmatron developed, three-phase ac circuit is used with three step-up transformers and three diode arms. The circuit makes it possible to conduct the operation of the magnetron in a continuous mode. In order to implement a pulse-periodic mode of magnetron operation, one of the diode arms in the circuit was switched off. For diagnostics of plasma generation in the jet we used floating potential measuring by oscilloscope, the probe of which was placed in the region of the cold plasma jet. In the continuous mode the floating potential oscillated weakly around a constant value which depends on the distance to the torch. It was found that the pulse-periodic mode was carried out with a frequency of 50 Hz and with a pulse duration of 15 ms. Formation of spark channels was observed. In the continuous mode spark discharges did not occur, and the discharges between the electrodes and the inner wall of the chamber were glow type. The work is supported by the Russian Foundation for Basic Research (grant No. 19-08-00844).

On the enthalpy flux in a plasma jet of nitrogen–argon mixture

Kulikov Yu M[1,@], Gadzhiev M Kh[1] and Son E E[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 141701, Russia

[@] kulikov-yurii@yandex.ru

Low-temperature plasma generators create a stream of highly ionized quasineutral gas which in some cases forms an immersed jet allowing to treat this process in a view of classical problems of fluid mechanics. Essential factors here are the nonequilibrium radiative cooling of the plasma leading to rapid quenching of macroscopic fluid particles, as well as the equilibrium recombination of atoms and molecules that changes the average molar mass of the mixture. For the immersed jet leaving the plasma torch, the composition and plasma enthalpy of the N_2 and Ar mixture were calculated based on the equations of dissociative and ionization equilibrium (Saha-type) taking into account the dissociation of nitrogen, and the sequential ionization reactions leading to the separation of all valence electrons from the outer shell of N and the appearance of multiply charged ions. The calculation of the enthalpy flux carried by the plasma jet, which is a mixture of nitrogen and argon at different flow ratios, showed that when the mass fraction of nitrogen is varied in the range of 1–10%, and the mass-average temperature can change by 3000 K. One can compare the enthalpy flux in a plasma jet (according to the flow rate data), effective power (according to the current–voltage characteristic), and also the corresponding temperatures with the results of spectroscopic measurements. To determine the specific heat fluxes of the plasma, calorimetric measurements of the heat fluxes removed by water were performed while cooling the cylindrical ends of the calorimeter from copper, where the central section was made of both copper and tungsten.

Emission spectra of atmospheric-pressure electrode microwave discharge in Ar and of cold plasma jet

Yusupov D I[1,@]**, Sargsyan M A**[1]**, Antipov S N**[2] **and Gadzhiev M Kh**[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Limited Company "AGNI-K", Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] yusupovdi@ihed.ras.ru

In the present work, the method of emission spectroscopy was used to study both Ar electrode microwave discharge in the external plasma torch developed for biomedical applications and afterglow plasma in cold plasma jet behind the torch outlet. The experimental setup based on the previously developed multipurpose atmospheric-pressure microwave plasmatron was used. The plasmatron operates at a frequency of 2.45 GHz, has a microwave power in the waveguide of up to 2.5 kW and a power in the torch of up to 200 W. The plasma torch consists of cylindrical common chamber of 2.5 cm outlet diameter with 6 rod-like electrodes forming a regular hexagon in a cross-section. Discharge channels are formed between the ends of the electrodes and the inner wall of the discharge chamber. In this case, the discharges are as close as possible to the torch outlet. Ar of high purity (99.998%) was used with the flow rate in the range from 0 to 10 standard liters per minute. In order to conduct spectral measurements, Avaspec 2048 three-channel spectrometer was used. Molecular lines of NO, OH, N_2, NH and atomic lines of Ar were found in the spectrum in the discharge channels. Based on the analysis of the spectra, it was shown that the translational plasma temperature in the discharge channel can reach 1500 K. In the cold plasma jet spectrum, due to its weak luminescence, only the molecular lines OH and N_2 were reliably observed. The work is supported by the Russian Foundation for Basic Research (grant No. 18-08-01312).

Ion composition of nitrogen plasma jet with carbon admixture

Kavyrshin D I[@], Chinnov V F, Sargsyan M A, Shcherbakov V V, Khromov M A and Korshunov O V

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

[@] dimakav@rambler.ru

With the aim of studying nitrogen plasma flow impacting graphite surfaces, we investigated the evolution of a plasma jet moving from the nozzle of the plasma torch to the target [1]. The motion is accompanied by a decrease in temperature from 10 to 7 kK [2] with a loss of $\approx 60\%$ of the deposited energy and an increase in the density of carbon-containing impurities with partial preservation of the local thermodynamic equilibrium. The main reactions are thermal processes of the formation and decomposition of molecules, dissociative recombination and recharging of nitrogen ions. In the presence of carbon impurities, this set is supplemented with the substitution reaction $C + N_2 \longleftrightarrow CN + N$, electron-collision processes of stepwise ionization and recombination, and a whole ion-molecular cascades of reloads and substitutions. It has been established that a small admixture of carbon ($\sim 0.1\%$) manifests itself only in ion-molecular kinetics, increasing the electron concentration, determining the ionic composition of the plasma, and thereby violating the equilibrium between its neutral and charged components. This leads, in particular, to the recombination nonequilibrium distribution of carbon atoms over electronic states. Other carbon-containing impurities (CN and C_2) are not significant.

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[2] Belevtsev A A, Kavyrshin D I, Sargsyan M A, Chinnov V F, Efimov A V and Shcherbakov V V 2019 *J. Phys. D: Appl. Phys.* **51** 484002

Composite material development for the single phase high voltage alternating current plasma torch

Dudnik Yu D[@], Safronov A A, Kuznetsov V E, Shiryaev V N and Vasilieva O B

Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, Russia

[@] julia_dudnik-s@mail.ru

The aim of this work is to develop composite materials that provide long-term and reliable operation of loaded elements of high-voltage ac plasmatrons [1, 2], including electrode blocks and insulation materials included in its design, capable of withstanding significant thermal loads. The plasma torch water cooling case is made of stainless steel, the gas supply is tangential. The electrodes are mounted through bushing insulators in the case channels, the nozzle is positioned in the other part of the channel. All these elements are subjected to high thermal load. They experience significant heat shock due to rapid heating by the plasma jet and intensive cooling by the gas stream. It can lead to the reduction of their operating life [3]. This paper presents some results of the performed researches. Various materials have been studied, including wireframe composite carbide materials containing copper and ceramic insulating materials based on organosilicon resins, to increase the life of the electrode blocks and insulating materials.

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Statistics of current pulses in a surface barrier discharge on electrodes of various materials

Selivonin I V[@] and Moralev I A

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

[@] inock691@ya.ru

Surface dielectric barrier discharge (sDBD) is used in numerous technological processes in the field of plasma chemistry, treatment of biological objects, and aerodynamics. In many cases, operational performance of devices based on DBD depends on the electrical characteristics of the discharge, which are determined the parameters of single microdischarges and their statistics. The mode of operating of the discharge strongly depends on the material of the corona electrode. So, in paper [1] it was demonstrated that in the case of a tungsten electrode, DBD looks like a diffuse glow region, in the case of a copper electrode, the discharge is non-uniform. Besides, in works [2, 3], it was shown that the formation of oxides on the corona edge leads to significant changes in the mode of operation of the discharge and its electrical characteristics. This work raises the question of the influence of electrode material and electrode edge state on the parameters of single pulses and their statistics. The temporal and spatial statistics of current pulses in a surface barrier discharge powered by an alternating sinusoidal voltage has been studied. The shape of "average" current pulses are obtained. Distributions of such characteristics as transferred charge, pulse duration are obtained. The existence of two types of microdischarges is demonstrated. A comparison of the data obtained for different types of electrodes.

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Pulse and electrodes polarity effects on pulsed electrical breakdown in microbubbly media

Panov V A[@], Vasilyak L M, Vetchinin S P, Pecherkin V Ya 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

Electrical breakdown reveals strong polarity effects in both gases and liquids [1, 2]. Even in electrodes geometry with quasi-uniform electric field distribution breakdown plasma channels developing from anode and cathode differ significantly from each other considering channel propagation speed, breakdown timing for each breakdown stage, geometry and structure of the channel, appeared luminosity. Polarity effect becomes even more prominent when coming to non-uniform electric field. Sharp electrode edges brings the stability to initiation of breakdown channel making it more reproducable and examinable. Electrical breakdown in conductive water and microbubbly media based on it has been studied extensively in last years [3] for positive polarity (pin-anode system). Thermal mechanism of breakdown in both liquids with and without bubbles has been revealed, as well as its transition to fast streame-leader breakdown mechanism and guidance effect of microbubbles in bulk liquid on developing plasma channel trajectory. With this work we study effects of both changing polarities of electrodes system and the pulsed voltage supplying and its uniq features posessed by microbubbly media.

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Winter rye tolerance to low temperatures after seed treatment with surface barrier discharge

Gundareva S V[1], Lazukin A V[1,2,@], Dorofeev N V[3], Romanov A G[1] and Krivov S A[1]

[1] National Research University Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia
[2] Timiryazev Institute of Plant Physiology of the Russian Academy of Sciences, Botanicheskaya 35, Moscow 127276, Russia
[3] Siberian Institute of Plant Physiology and Biochemistry of the Siberian Branch of the Russian Academy of Sciences, Lermontov Street 132, Irkutsk 664033, Russia

[@] lazukin_av@mail.ru

Presowing treatment of seeds of agricultural crops by gas-discharge low-temperature plasma products is one of the promising methods for increasing plant productivity [1]. In this work, the experimental results of surface barrier discharge plasma products affection to winter rye seed germination at the initial stage of growth and seedling tolerance to low temperatures are shown. The treatment was carried out for 10, 60, and 180 s in the plane-parallel electrode system with sinusoidal voltage of 2.7 kV with frequency 4.4 kHz applied to the strip electrodes at a distance of 5 mm from each other. It is shown that the treatment has no effect on seed germination. Also a tendency to the seedling relative freeze tolerance increase in 60 and 180 s exposure treatment modes is shown. In 180 s exposure treatment mode, the stimulation of 3-day seedling shoot and root system length also occurs. The freeze tolerance increase relative to control samples occurs only with freezing at temperatures of -18 and -20 °C.

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Particle-in-cell simulation of the ion beam propagation in electro-magnetic field for plasma separation

Smirnov V S[1,2,@]**, Egorov R O**[1,2]**, Gavrikov A V**[1,2] **and Kislenko S A**[1,2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] smvl95@mail.ru

Spent nuclear fuel recycle is an economic and environmental issue in nuclear power engineering. To improve the situation plasma separation method is being rapidly developed. In this work, we propose particle-in-cell simulation [1] in a single-particle approximation of ions spatial separation in a plasma separator Laplace 1 [2]. A cylindrically symmetric electric field obtained in the work [3] was used. Magnetic field heterogeneity was taken into account. The model ion beam injected into the separator imitates ionized spent uranium nuclear fuel containing U-235 ions and fission products with a mass distribution corresponding to thermal neutron fission of U-235. The injected ions had a variable energy range (1–20 eV) and angle spread of the initial ion velocities. The goal of our work is to improve the separation of a heavy fraction (U-235) by searching for optimal initial energy range, angle spread of the ion beam, magnetic field value, optimal injection region for the ion beam. We obtain that the best injection region for the effective separation of the ions heavy fraction with a mass of U-235 are the planes $z = 0$ and -0.5 m. We show that an important parameter for ion separation is the distance from the injection site to the separator axis. Besides an increase in the magnetic field leads to a better separation of the heavy fraction.

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ORGANIZATION LIST

12CSRI MOD RF — 12 Central Scientific Research Institute of the Ministry of Defense of the Russian Federation, Sergiev Posad, Moscow Region 141307, Russia

BelgSTU, NB — Novorossiysk Branch of the Shukhov Belgorod State Technological University, Mysknakskoye Shosse 75, Novorossiysk, Krasnodar Region 353919, Russia

BMSTU — Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow 105005, Russia

CCFE, UKAEA — Culham Centre for Fusion Energy, United Kingdom Atomic Energy Authority, Culham Science Centre, Abingdon, Oxfordshire OX143EB, United Kingdom (Great Britain)

Chepan — Private Entrepreneur in Science, Lenina 19-3, Sevastopol 299011, Russia

CI RAS — Ibragimov Complex Institute of the Russian Academy of Sciences, Staropromyslovsky Avenue 21a, Grozny, Chechen Republic 364051, Russia

CIAM — Central Institute of Aviation Motors, Aviamotornaya Street 2, Moscow 111116, Russia

DSU — Dagestan State University, Magomeda Gadzhieva 43a, Makhachkala, Dagestan 367000, Russia

FiratUni — Firat University, Elazig 23169, Turkey

FRCCP RAS — Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, Kosygina Street 4, Moscow 119991, Russia

FSRC CP RAS — Federal Scientific Research Centre "Crystallography and Photonics" of the Russian Academy of Sciences, Leninsky Avenue 59, Moscow 119333, Russia

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

HSE — National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

IAM RAS — Institute of Applied Mechanics of the Russian Academy of Sciences, Leninsky Avenue 32a, Moscow 117334, 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

IEC SB RAS — Institute of the Earth's Crust of the Siberian Branch of the Russian Academy of Sciences, Lermontov Street 128, Irkutsk 664033, Russia

IEE RAS — Institute for Electrophysics and Electrical Power of the Russian Academy of Sciences, Dvortsovaya Naberezhnaya 18, Saint-Petersburg 191186, 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

IGRRE JIHT RAS — Institute for Geothermal Research and Renewable Energy—Branch of the Joint Institute for High Temperatures of the Russian Academy of Sciences, Shamilya 39a, Makhachkala, Dagestan 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

IKI RAS — Space Research Institute of the Russian Academy of Sciences, Profsoyuznaya 84/32, Moscow 117997, Russia

IMP UB RAS — Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, Sofya Kovalevskaya Street 18, Ekaterinburg 620219, Russia

INR RAS — Institute for Nuclear Research of the Russian Academy of Science, Prospekt 60-letiya Oktyabrya 7a, Moscow 117312, Russia

IoffeInst — Ioffe Institute, Polytekhnicheskaya 26, Saint-Petersburg 194021, Russia

IPCET SB RAS — Institute for Problems of Chemical and Energetic Technologies of the Siberian Branch of the Russian Academy of Sciences, Sotsialisticheskaya 1, Biysk, Altayskiy Kray 659322, 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 61, Saint-Petersburg 199178, Russia

IPP RAS — Timiryazev Institute of Plant Physiology of the Russian Academy of Sciences, Botanicheskaya 35, Moscow 127276, Russia

ISSP RAS — Institute of Solid State Physics of the Russian Academy of Sciences, Akademika Osipyana Street 2, Chernogolovka, Moscow Region 142432, Russia

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

ITMOU — ITMO University, Kronvergskiy 49, Saint-Petersburg 197101, 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 Sciences, Akademika Semenova 1a, Chernogolovka, Moscow Region 142432, Russia

ITP UB RAS — Institute of Thermal Physics 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

JINR — Joint Institute for Nuclear Research, Zholio-Kyuri 6, Dubna, Moscow Region 141980, Russia

KBSC RAS — Kabardino-Balkar 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 Street 18, Kazan, Tatarstan 420008, Russia

KIAM RAS — Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, Miusskaya Square 4, Moscow

125047, Russia

KNRTU — Kazan National Research Technological University, Karl Marx Street 68, Kazan, Republic of Tatarstan 420015, Russia

KNRTU-KAI — Kazan National Research Technical University named after A N Tupolev—KAI, Karl Marx Street 10, Kazan, Tatarstan 420111, 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

LPI RAS — Lebedev Physical Institute of the Russian Academy of Sciences, Leninsky Avenue 53, Moscow 119991, Russia

MAI — Moscow Aviation Institute, Volokolamskoe Shosse 4, Moscow 125993, Russia

MIPT — Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

MISIS — National University of Science and Technology "MISIS", Leninskiy Avenue 4, Moscow 119049, Russia

MUCTR — Mendeleev University of Chemical Technology of Russia, Miusskaya Square 9, Moscow 125047, Russia

NKJ — Science and Life Magazine, Myasnitskaya 27/7 Bldg 1, Moscow 101000, 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

OGRI RAS — Oil and Gas Research Institute of the Russian Academy of Sciences, Gubkin Street 3, Moscow 119991, Russia

Osaka University, ILE — Institute of Laser Engineering, Osaka University, 2-6 Yamadaoka, Suita, Osaka 565-0871, Japan

RSREU — Ryazan State Radio Engineering University, Gagarin Street 59/1, Ryazan 390005, Russia

RTU MIREA — MIREA—Russian Technological University, Vernadskogo Avenue 78, Moscow 119454, Russia

RUSAL — United Company RUSAL, Vasilisy Kozhinoy Street 1, Moscow 121096, Russia

Skoltech — Skolkovo Institute of Science and Technology, Skolkovo Innovation Center Bldg 3, Moscow 143026, Russia

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

SPbSTU — Saint-Petersburg State Technological Institute (Technical University), Moskovsky Avenue 26, Saint-Petersburg 190013, Russia

SPbSU — Saint-Petersburg State University, Universitetskaya Naberezhnaya 7/9, Saint-Petersburg 199034, Russia

SRC RF TRINITI — State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia

SSC RF FSUE KRC — State Scientific Centre of the Russian Federation—Federal State Unitary Enterprise Keldysh Research Center, Onezhskaya Street 8, Moscow 125438, Russia

SUSU — South Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia

TSTU — Tambov State Technical University, Sovetskaya Street 106, Tambov 392000, Russia

UNC — National University of Cordoba, Avenue Velez Sarsfield 1611, Cordoba X5000, Argentina

UPC — Universitat Politecnica de Catalunya, BarcelonaTech, C. Jordi Girona, 31, Barcelona 08034, Spain

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

VNIIA(L) — Dukhov Research Institute of Automatics (VNIIA), Luganskaya 9, Moscow 115304, Russia

VNIIA(S) — Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya 22, Moscow 127055, Russia

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

PARTICIPANT LIST

1. *Adiguzel Osman*, FiratUni, +90(536)5638403, oadiguzel@hotmail.com
2. *Akhmatov Zeitun Anuarovich*, KBSU, ahmatov.z@bk.ru
3. *Alekseev Vladimir Viktorovich*, FSUE RFNC–VNIIEF, chmel.ru@mail.ru
4. *Alekseevskaya Anastasia Aleksandrovna*, JIHT RAS, anastasiya.alekseevskaya@phystech.edu
5. *Alikhanov Ibragim*, INR RAS, +7(866)3875221, ialspbu@gmail.com
6. *Alkhimova Mariya Andreevna*, JIHT RAS, MAAlkhimova@mephi.ru
7. *Ananev Sergei Yurevich*, JIHT RAS, serg.ananev@gmail.com
8. *Andreev Nikolay Evgen'evich*, JIHT RAS, andreev@ras.ru
9. *Anisichkin Vladimir Fedorovich*, LIH SB RAS, avf@hydro.nsc.ru
10. *Antropov Aleksandr Sergeevich*, JIHT RAS, antropov@phystech.edu
11. *Apfelbaum Evgeny Mikhailovich*, JIHT RAS, +7(495)4844433, apfel_e@mail.ru
12. *Arkar Kyaw*, MIPT, akarkyaw53@gmail.com
13. *Badretdinova Leisan Kharisovna*, KNRTU, badretdinova_kstu@mail.ru
14. *Baidakov Vladimir Georgievich*, ITP UB RAS, +7(343)2678806, bai@itp.uran.ru
15. *Baidin Ivan Sergeevich*, LPI RAS, ibaydin@yandex.ru
16. *Bakulin Ivan Konstantinovich*, JIHT RAS, bakulin.ik@phystech.edu
17. *Bakulin Vladimir Nikolaevich*, IAM RAS, vbak@yandex.ru
18. *Baldin Anton Aleksandrovich*, JINR, an.baldin@mail.ru
19. *Baldina Elina Georgievna*, JINR, e.baldina@mail.ru
20. *Bardina Tatiana Leonidovna*, JIHT RAS, bardina_1994@mail.ru
21. *Barenbaum Azariy Aleksandrovich*, OGRI RAS, +7(495)4842456, azary@mail.ru
22. *Barsukova Anastasiia Aleksandrovna*, JIHT RAS, anastasiya.barsukova@phystech.edu

23. *Bayandin Yuriy Vitalievich*, ICMM UB RAS, buv@icmm.ru
24. *Bazarov Yuri Borisovich*, FSUE RFNC–VNIIEF,
    +7(83130)20223, johnub.silver@gmail.com
25. *Belikov Roman Sergeevich*, JIHT RAS, ihatepesh@mail.ru
26. *Bisti Veronika Evgenievna*, ISSP RAS, bisti@issp.ac.ru
27. *Bobrov Andrei Alexandrovich*, JIHT RAS, abobrov@inbox.ru
28. *Bobrov Viktor Borisovich*, JIHT RAS, vic5907@mail.ru
29. *Bogomaz Alexander Alekseevich*, IEE RAS,
    +7(812)13151757, bogomazal@rambler.ru
30. *Bratov Vladimir*, IPME RAS, vladimir@bratov.com
31. *Bugay Irina Vladimirovna*, MAI, irinbug@yandex.ru
32. *Burov Arseniy Sergeevich*, MIPT, burov.as@phystech.edu
33. *Buyko Anatoly Mikhailovich*, FSUE RFNC–VNIIEF,
    +7(83130)44740, AMBuyko@vniief.ru
34. *Byalko Alexey Vladimirovich*, ITP RAS, alex@byalko.ru
35. *Bystrov Nikita Sergeevich*, JIHT RAS,
    bystrovns.jiht@gmail.com
36. *Bystryi Roman*, HSE, broman.meld@gmail.com
37. *Chepan Oleg Bronislavovich*, Chepan, eksmm15@mail.ru
38. *Chepelev Vladimir Mikhailovich*, JIHT RAS,
    chepelev@ihed.ras.ru
39. *Cheprunov Alexander Alexandrovich*, 12CSRI MOD RF,
    alexander.cheprunov@yandex.ru
40. *Chigvintsev Alexander Yurievich*, MIPT,
    alex012008@gmail.com
41. *Chistolinov Andrey Vladimirovich*, JIHT RAS,
    a-chi@yandex.ru
42. *Chugunov Andrey Igorevich*, IoffeInst,
    andr.astro@mail.ioffe.ru
43. *Deminsky Maxim Alexandrovich*, NRC KI, +7(499)1967362,
    deminskiy_ma@nrcki.ru
44. *Deputatova Lidiya Viktorovna*, JIHT RAS, +7(495)4842429,
    dlv@ihed.ras.ru
45. *Dolgov Evgeniy Vladimirovich*, JIHT RAS,
    triumph9311@gmail.com
46. *Dolnikov Gennady Gennadjevich*, IKI RAS, dolnikov@mail.ru
47. *Dudin Sergey Vasilyevich*, IPCP RAS, +7(496)5225168,
    dudinsv@ficp.ac.ru
48. *Dudnik Yuliya Dmitrievna*, IEE RAS, +7(812)5715383,

julia_dudnik-s@mail.ru

49. *Dyachkov Lev Gavriilovich*, JIHT RAS, +7(495)3625310, dyachk@mail.ru
50. *Dyachkov Sergey*, VNIIA(S), serj.dyachkov@gmail.com
51. *Dzhapparov Tamerlan Absalam-Gadzhievich*, IGRRE JIHT RAS, timur507@mail.ru
52. *Dzlieva Elena Soslanovna*, SPbSU, +7(812)4284466, plasmadust@yandex.ru
53. *Efimchenko Vadim Sergeevich*, ISSP RAS, +7(496)5228410, efimchen@issp.ac.ru
54. *Efremov Vladimir Petrovich*, JIHT RAS, +7(495)4850963, dr.efremov@gmail.com
55. *Egorov Kirill Sergeevich*, BMSTU, blackbird05@mail.ru
56. *Elyanov Artem Evgenievich*, JIHT RAS, elyanov14@physics.msu.ru
57. *Emelianov Alexander Valentinovich*, JIHT RAS, +7(495)4841966, aemelia@ihed.ras.ru
58. *Emelyanov Andrey Nikolaevich*, IPCP RAS, emelyanov@ficp.ac.ru
59. *Eremin Alexander*, JIHT RAS, +7(495)4832314, eremin@ihed.ras.ru
60. *Erunov Sergey Vladimirovich*, FSUE RFNC–VNIIEF, pakucherova@mail.ru
61. *Fairushin Ilnaz Izailovich*, JIHT RAS, fairushin_ilnaz@mail.ru
62. *Faleeva Yulia Mikhailovna*, JIHT RAS, faleeva.julia@mail.ru
63. *Fedorov Ilya Dmitrievich*, JIHT RAS, ilya.d.fedorov@phystech.edu
64. *Fedotov Anton Andreevich*, NRU MPEI, monolitk3@gmail.com
65. *Ferreyra Ricardo Toms*, UNC, +54(351)5581455, ricardotf45@hotmail.com
66. *Filinov Vladimir Sergeevich*, JIHT RAS, vladimir_filinov@mail.ru
67. *Filippov Anatoly Vasilievich*, JIHT RAS, fav@triniti.ru
68. *Fleita Dmitrii*, HSE, momysf@gmail.com
69. *Fokin Vladimir Borisovich*, JIHT RAS, +7(495)4842456, vladimir.fokin@phystech.edu
70. *Fortov Vladimir Evgenievich*, JIHT RAS, +7(495)4857988, konst@ihed.ras.ru

71. *Gadzhiev Makhach Khairudinovich*, JIHT RAS, makhach@mail.ru
72. *Galimzyanov Bulat Nailevich*, KFU, bulatgnmail@gmail.com
73. *Galiullin Igor Gaptilbarievich*, FSUE RFNC–VNIITF, galiullin-igor@mail.ru
74. *Gangapshev Albert Musaevich*, INR RAS, gangapsh@list.ru
75. *Gavrikov Andrey Igorevich*, NRC KI, gavrikovandrey@yandex.ru
76. *Glushneva Alexandra Vladimirovna*, MIPT, glushniova.alexandra@gmail.com
77. *Godina Ekaterina Petrovna*, IEE RAS, godina-ekaterina@mail.ru
78. *Goldshtein Klim Dmitrievich*, MIPT, kgoldm19@gmail.com
79. *Golovin Daniil*, Osaka University, ILE, +81(80)91291497, golovin-d@ile.osaka-u.ac.jp
80. *Gongora Rincon Julian Gonzalo*, UNC, +54(351)6120510, jgongoramates@gmail.com
81. *Gorbachev Valery Vladimirovich*, INR RAS, +7(86638)7504, vvgor_gfb1@mail.ru
82. *Gordeev Ilia Sergeevich*, JIHT RAS, gordeevilu@gmail.com
83. *Gordeev Vladimir*, IPCET SB RAS, +7(3854)301866, gordeev.vladimir92@yandex.ru
84. *Gorokhov Sergey Aleksandrovich*, FSUE RFNC–VNIITF, +7(35146)51180, dep5@vniitf.ru
85. *Gribov Iourii Aronovich*, ITNE, +7(499)7264769, jgribov@yandex.ru
86. *Grigoryev Vladislav Vladimirovich*, JIHT RAS, grigoriev.vl.vl@yandex.ru
87. *Grishin Leonid Igorevich*, JIHT RAS, lenya-grishin@mail.ru
88. *Gurtovoy Sergey Antovovich*, RUSAL, sergey.gurtovoy@phystech.edu
89. *Ignatova Olga Nikolaevna*, FSUE RFNC–VNIIEF, +7(831)3022401, onignatova@gmail.com
90. *Inogamov Nail*, ITP RAS, nailinogamov@gmail.com
91. *Iosilevskiy Igor L'vovich*, JIHT RAS, iosilevskiy@gmail.com
92. *Iurin Vadim Petrivich*, CIAM, Iurin@rtc.ciam.ru
93. *Ivanov Artyom Vladislavovich*, JIHT RAS, avivanov_2@edu.hse.ru
94. *Kadatskiy Maxim Alekseevich*, JIHT RAS,

makkad@yandex.ru

95. *Karpov Maxim Alexandrovich*, FSUE RFNC–VNIIEF, maksim.karpov@gmail.com
96. *Karpov Stanislav Alexandrovich*, VNIIA(S), karpov.st@yandex.ru
97. *Kaufman Sergey Victorovich*, MIPT, wolf.reborn@mail.ru
98. *Kavyrshin Dmitry Igorevich*, JIHT RAS, dimakav@rambler.ru
99. *Kazanskiy Pavel Nikolaevich*, JIHT RAS, fokkoo@yandex.ru
100. *Kaziev Andrey Victorovich*, NRNU MEPhI, +7(495)7885699, avkaziev@gmail.com
101. *Kazieva Tatiana Vadimovna*, NRNU MEPhI, glizerogen@gmail.com
102. *Khabibrakhmanov Almaz Ildarovich*, MISIS, almaz.khabibrakhmanov@phystech.edu
103. *Khirianova Alexandra Igorevna*, LPI RAS, khirianova.alexandra@gmail.com
104. *Khishchenko Konstantin Vladimirovich*, JIHT RAS, +7(495)4842483, konst@ihed.ras.ru
105. *Khokhlov Victor Alexandrovich*, ITP RAS, v_a_kh@mail.ru
106. *Khokonov Azamat Khazret-Alievich*, KBSU, azkh@mail.ru
107. *Khokonov Murat Khazretalievich*, KBSU, khokon6@mail.ru
108. *Khromova Elena Sergeevna*, IPCP RAS, +7(496)5224471, lsk@icp.ac.ru
109. *Khusnutdinoff Ramil Minnegayazovich*, KFU, khrm@mail.ru
110. *Kim Dmitriy Andreevich*, KIAM RAS, dima83ipm@yandex.ru
111. *Kireeva Anna*, JIHT RAS, redtvt@gmail.com
112. *Kirillova Alina Alekseevna*, SPbSTU, Feoctista-2016@yandex.ru
113. *Kirilyuk Vasily Alekseevich*, CIAM, kiriluk.94@yandex.ru
114. *Klenov Alexander Ivanovich*, FSUE RFNC–VNIITF, Klenov174@gmail.com
115. *Kliavinek Sergey Sergeevich*, JIHT RAS, klyavinekss@gmail.com
116. *Klinacheva Nataliia Leonidovna*, SUSU, klinachevanl@susu.ru
117. *Kochkarov Makhti*, INR RAS, +7(866)3875221, makhti.kochkarov@yandex.ru
118. *Kochnev Dmitry Mikhailovich*, SRC RF TRINITI, dimich17@mail.ru
119. *Kolesnikov Petr Aleksandrovich*, FSUE RFNC–VNIITF,

kolesnikov.peter@mail.ru

120. *Kolotilov Vadim Alexeyevich*, ITAM SB RAS,
kolotilov1992@gmail.com

121. *Kolotushkin Roman Nikolaevich*, JIHT RAS,
kolotushkin.roman@gmail.com

122. *Komarov Pavel Sergeevich*, JIHT RAS, +7(495)2294240,
komarov-p@yandex.ru

123. *Komissarov Pavel Vladimirovich*, FRCCP RAS,
dot-dot@inbox.ru

124. *Kondratyev Arseniy Mikhailovich*, JIHT RAS,
cpl593h@mail.ru

125. *Kondratyuk Nikolay Dmitrievich*, HSE, nkondratyuk@hse.ru

126. *Kononov Evgenii Alexandrovich*, JIHT RAS,
GADvin@yandex.ru

127. *Konyukhov Andrey Viktorovich*, JIHT RAS,
konyukhov_av@mail.ru

128. *Korneev Boris Azamatovich*, KIAM RAS,
boris.korneev@phystech.edu

129. *Korneva Maria Andreevna*, Skoltech,
marijakorneva@yandex.ru

130. *Korobeynikov Igor Vital'yevich*, IMP UB RAS,
+7(343)3783779, i_korobeynikov@mail.ru

131. *Korotaev Pavel*, VNIIA(S), +7(499)9787803,
korotaev.py@mipt.ru

132. *Korshunova Maya*, JIHT RAS,
ekaterina.mikheyeva@gmail.com

133. *Kostanovskiy Alexander Viktorovich*, JIHT RAS,
+7(495)3625123, kostanovskiy@gmail.com

134. *Kozharin Alexey Sergeevich*, JIHT RAS, +7(495)4842456,
1alekseik1@gmail.com

135. *Krasnova Polina Andreevna*, JIHT RAS, +7(495)4842456,
pakrasnova@gmail.com

136. *Kravchenko Igor Vitalyevich*, IPCP RAS, +7(495)5221447,
krav@ficp.ac.ru

137. *Kreopalov Dmitrii Vladislavovich*, BMSTU, +7(495)5632322,
dkreopalov@mail.ru

138. *Krikunova Anastasiia Igorevna*, MIPT,
krikunovaai@gmail.com

139. *Krivosheev Sergey Ivanovich*, SPbPU, ksi.mgd@gmail.com

140. *Kuchko Dmitriy*, FSUE RFNC–VNIITF, kdp007@mail.ru
141. *Kudryavtsev Andrey Vladimirovich*, RTU MIREA, oldousavk@yandex.ru
142. *Kudryavtseva Irina Vladimirovna*, ITMOU, togg1@yandex.ru
143. *Kulikov Yury Matveevich*, JIHT RAS, kulikov-yurii@yandex.ru
144. *Kulish Mikhail Ivanovich*, IPCP RAS, kulishm@ficp.ac.ru
145. *Kurilenkov Yuri Konstantinovich*, JIHT RAS, +7(495)4841647, kurilenkovyuri@gmail.com
146. *Kuzmin Sergey Nikolaevich*, TSTU, +7(4752)630446, penergy@list.ru
147. *Kuzmina Julia Sergeevna*, JIHT RAS, juli_kuzmina@mail.ru
148. *Kuznetsov Sergey Dmitrievich*, FSUE RFNC–VNIIEF, +7(83130)44740, SDKuznetsov@vniief.ru
149. *Kuznetsov Sergey Vyacheslavovich*, JIHT RAS, +7(495)4859722, shenau@rambler.ru
150. *Kyarov Aslan Khasanovich*, KBSU, pnr@kbsu.ru
151. *Lankin Alexander Valerievich*, JIHT RAS, Alex198508@yandex.ru
152. *Larkin Alexander Sergeevich*, JIHT RAS, alexanderlarkin@rambler.ru
153. *Lavrenov Vladimir Alexandrovich*, JIHT RAS, v.a.lavrenov@gmail.com
154. *Lavrinenko Yaroslav*, JIHT RAS, lavrinenko@phystech.edu
155. *Lazukin Alexandr Vadimovich*, IPP RAS, lazukin_av@mail.ru
156. *Lenev Dmitrii Yurevich*, JIHT RAS, lenevdy@mail.ru
157. *Levashov Pavel Remirovich*, JIHT RAS, +7(495)4842456, pasha@jiht.ru
158. *Li Elena Sergeevna*, NKJ, yes.li@mail.ru
159. *Likhachev Aleksandr Pavlovich*, JIHT RAS, +7(495)4842338, apl@ihed.ras.ru
160. *Lisin Evgeny*, JIHT RAS, eaLisin@yandex.ru
161. *Lisina Irina*, JIHT RAS, +7(495)4842355, irina.lisina@mail.ru
162. *Loginova Anna Andreevna*, CIAM, loginova.aa@yandex.ru
163. *Logunov Mikhail Alexandrovich*, JIHT RAS, mikhail.logunov@phystech.edu
164. *Loktionov Egor Yuryevitch*, BMSTU, yagor@bmstu.ru
165. *Lukin Alexander Nikolayevitch*, WCRC, lukin@wcrc.ru
166. *Lunev Artem*, CCFE, UKAEA, +44(0)1235464358,

artem.lunev@ukaea.uk

167. *Lutovinov Alexander Anatolyevich*, IKI RAS, aal@iki.rssi.ru
168. *Maiorov Sergey Alekseevich*, GPI RAS, mayorov_sa@mail.ru
169. *Makarov Sergey Stanislavovich*, JIHT RAS, +7(495)4841944, seomakarov28@gmail.com
170. *Maltsev Maxim Alexandrovich*, JIHT RAS, daerus21@yandex.ru
171. *Malyshev Andrey Nikolaevich*, FSUE RFNC–VNIIEF, starmen74@mail.ru
172. *Markina Elena*, JIHT RAS, lenmarkina@gmail.com
173. *Martynenko Artem Sergeevich*, JIHT RAS, artmarty@mail.ru
174. *Martynova Inna Aleksandrovna*, JIHT RAS, +7(495)4842300, martina1204@yandex.ru
175. *Medvedev Mikhail Andreevich*, LPI RAS, mihail.medvedev@phystech.edu
176. *Melnikov Anton Dmitrievich*, JIHT RAS, antonmelnikoff@yandex.ru
177. *Melnikova Kseniya Sergeevna*, JIHT RAS, mkss-ks@yandex.ru
178. *Mikhaylov Vadim Nikolaevich*, FSUE RFNC–VNIITF, v.n.mikhaylov@vniitf.ru
179. *Mikheyeva Ekaterina*, JIHT RAS, ekaterina.mikheyeva@gmail.com
180. *Mikushkin Anton Yuryevich*, JIHT RAS, notna17@yandex.ru
181. *Minakov Dmitry Vyacheslavovich*, JIHT RAS, +7(495)4842456, minakovd@ihed.ras.ru
182. *Miroshnichenko Taisia*, LPI RAS, taisia.miroshnichenko@gmail.com
183. *Mishin Aleksey Vladimirovich*, ITAM SB RAS, alekseymishin1994@gmail.com
184. *Mishina Elena Dmitrievna*, RTU MIREA, mishina_elena57@mail.ru
185. *Mkrtychev Oleg Vitalievich*, BelgSTU, NB, +7(8617)221333, oleg214@ya.ru
186. *Mochalov Mikhail Alekseevich*, FSUE RFNC–VNIIEF, +7(83130)22165, mcleodjr@mail.ru
187. *Mochalova Valentina*, IPCP RAS, roxete20000@mail.ru
188. *Mokshin Anatoly Vasilievich*, KFU, anatolii.mokshin@mail.ru
189. *Molchanov Dmitry Anatolyevich*, JIHT RAS,

dmitriy.molchanov13@gmail.com

190. *Molkov Sergey Vladimirovich*, IKI RAS, +7(495)3332222, molkov@cosmos.ru

191. *Morozova Tatiana Igorevna*, IKI RAS, timoroz@yandex.ru

192. *Nazarov Maxim Michailovich*, NRC KI, nazarovmax@mail.ru

193. *Negodin Vladislav Dmitrievich*, JIHT RAS, vdnegodin@gmail.com

194. *Nikolaev Dmitriy Nikolaevich*, IPCP RAS, nik@ficp.ac.ru

195. *Nikolskiy Vsevolod Pavlovich*, HSE, thevsevak@gmail.com

196. *Nizovtseva Irina*, UrFU, nizovtseva.irina@gmail.com

197. *Norman Genri Edgarovich*, JIHT RAS, genri.norman@gmail.com

198. *Novikov Leontiy Aleksandrovich*, SPbSU, +7(812)4284466, leontiy.novikov@gmail.com

199. *Obruchkova Liliya Rimovna*, JIHT RAS, o_liliya@ihed.ras.ru

200. *Obzhirov Anatoly Evgenievich*, JIHT RAS, obzhirov.ae@phystech.edu

201. *Oginov Alexander Vladimirovich*, LPI RAS, oginov@lebedev.ru

202. *Olkhovskiy Andrey Vladimirovich*, FSUE RFNC–VNIITF, OIG_63@list.ru

203. *Orekhov Maksim Aleksandrovich*, JIHT RAS, maksim.orekhov@phystech.edu

204. *Oreshkin Evgeny Vladimirovich*, LPI RAS, Oreshkin@lebedev.ru

205. *Oreshkin Vladimir Ivanovich*, IHCE SB RAS, oreshkin@ovpe.hcei.tsc.ru

206. *Orlova Yuliia Vladimirovna*, MIPT, juliaov00@gmail.com

207. *Osmanova Badzhihanum Kamilevna*, IGRRE JIHT RAS, badji@mail.ru

208. *Ostrik Afanasy Victorovich*, IPCP RAS, ostrik@ficp.ac.ru

209. *Ovechkin Anton Aleksandrovich*, FSUE RFNC–VNIITF, ovechkin.an@mail.ru

210. *Pankratov Pavel Aleksandrovich*, JIHT RAS, pankratov_pav@mail.ru

211. *Panov Vladislav*, JIHT RAS, +7(495)4858063, panovvladislav@gmail.com

212. *Papyrin Pavel Vitalievich*, BMSTU, +7(499)2636409, papyrin_pv@bmstu.ru

213. *Paramonov Mikhail Anatol'evich*, JIHT RAS, mikhail.a.paramonov@phystech.edu
214. *Parkevich Egor Vadimovich*, LPI RAS, parkevich@phystech.edu
215. *Patlazhan Stanislav*, FRCCP RAS, sapat@yandex.ru
216. *Pautov Andrey Alexeevich*, SRC RF TRINITI, pautov@phystech.edu
217. *Pavlov Sergei Ivanovich*, SPbSU, sergey_pavlov86@mail.ru
218. *Pecherkin Vladimir Yakovlevich*, JIHT RAS, +7(495)4841810, vpecherkin@yandex.ru
219. *Perfilyeva Anna Vladimirovna*, MUCTR, perfilyevaav@yandex.ru
220. *Petrik Galina Georgievna*, IGRRE JIHT RAS, galina_petrik@mail.ru
221. *Petrov Dmitriy Vitalievich*, FSUE RFNC–VNIITF, snzjones@mail.ru
222. *Petrov Yuri Vasilievich*, ITP RAS, uvp49@mail.ru
223. *Petrovskiy Victor Pavlovich*, JIHT RAS, +7(495)4859155, b1p2a3@mail.ru
224. *Petrunina Ekaterina Mikhailovna*, NRC KI, lozben@kintechlab.com
225. *Petukhov Evgeniy Alexandrovich*, FSUE RFNC–VNIITF, ea_petukhov@mail.ru
226. *Pinchuk Mikhail Ernestovich*, IEE RAS, pinchme@mail.ru
227. *Pletnev Alexander Evgenyevich*, JIHT RAS, sanya.pletniov@yandex.ru
228. *Pogosyan Petros Zorikovich*, ISSP RAS, pogosyanpz@gmail.com
229. *Pokatashkin Pavel Alexandrovich*, VNIIA(S), p.a.pokatashkin@gmail.com
230. *Polyachenko Yury Anatolievich*, MIPT, polyachenko.yua@phystech.edu
231. *Polyakov Dmitry Nikolaevich*, JIHT RAS, +7(495)4842610, cryolab@ihed.ras.ru
232. *Popel Sergey Igorevich*, IKI RAS, serg.i.popel@gmail.com
233. *Popov Vyacheslav Sergeevich*, JIHT RAS, slavapopov1991@yandex.ru
234. *Poptsov Aleksandr Germanovich*, FSUE RFNC–VNIITF, f-d-f@mail.ru

235. *Potapov Denis Olegovich*, MIPT, potapov.do@phystech.edu
236. *Povarnitsyn Mikhail*, JIHT RAS, +7(495)4842456, povar@ihed.ras.ru
237. *Privalov Petr Andreevich*, JIHT RAS, +7(495)4841810, petr.priv@gmail.com
238. *Prokoshin Artem Vladislavovich*, ISSP RAS, prokoshin.artem@gmail.com
239. *Protsenko Sergey Pavlovich*, ITP UB RAS, sp@itp.uran.ru
240. *Pudova Yana Dmitrievna*, JIHT RAS, pudova.y.d@mail.ru
241. *Ragimkhanov Gadzhimirza Balaglanovich*, DSU, gb-r@mail.ru
242. *Rakhel Anatoly Dmitrievich*, JIHT RAS, rakhel@oivtran.ru
243. *Razmyslov Alexander*, IPCP RAS, sanaraz@mail.ru
244. *Redondo Jose Manuel*, UPC, +34(93)631817127, jose.manuel.redondo@upc.edu
245. *Rekhviashvili Sergo*, KBSC RAS, rsergo@mail.ru
246. *Reshetniak Olga Borisovna*, SRC RF TRINITI, obr@triniti.ru
247. *Reshetniak Viktor Vitalyevich*, SRC RF TRINITI, viktor.reshetnyak84@gmail.com
248. *Rodin Mikhail Maximovich*, JIHT RAS, mikhail.rodin@phystech.edu
249. *Romanenko Viktor*, INR RAS, vsrom94@gmail.com
250. *Roshchin Dmytriy Evgenievich*, MIPT, roschin.d.e@mail.ru
251. *Rubtsov Ivan Andreevich*, LIH SB RAS, rubtsov@hydro.nsc.ru
252. *Rudina Anisa Khalilovna*, FSUE RFNC–VNIITF, anisarudina@gmail.com
253. *Rusin Sergey Petrovich*, JIHT RAS, +7(495)3620778, sprusin@yandex.ru
254. *Ryazantsev Sergey Nikolayevich*, NRU MPEI, sergryaz@mail.ru
255. *Rykounov Alexey Alexandrovich*, FSUE RFNC–VNIITF, arykounov@gmail.com
256. *Rykov Sergey Vladimirovich*, ITMOU, togg1@yandex.ru
257. *Rykov Vladimir Alekseevich*, ITMOU, togg1@yandex.ru
258. *Saakyan Sergey Aramovich*, JIHT RAS, saasear@gmail.com
259. *Safronov Konstantin Vladimirovich*, FSUE RFNC–VNIITF, konstantin.safronov@gmail.com
260. *Saikhanov Musa Baudinovich*, CI RAS,

saikhanov_musa@mail.ru

261. *Saitov Ilnur*, JIHT RAS, saitovilnur@gmail.com
262. *Sametov Eduard*, JIHT RAS, sametov@phystech.edu
263. *Samokhin Alexandr Anatolievich*, SRC RF TRINITI, +7(495)8518684, samokhin@triniti.ru
264. *Samokhvalov Andrey Alexandrovich*, ITMOU, samokhvalov.itmo@gmail.com
265. *Sargsyan Mikael Armenovich*, JIHT RAS, m.sargsyan86@mail.ru
266. *Sartan Roman Alexandrovich*, JIHT RAS, r.sartan@gmail.com
267. *Satonkina Nataliya Petrovna*, LIH SB RAS, snp@hydro.nsc.ru
268. *Savintsev Alexey Petrovich*, KBSU, +7(8662)423777, savinal@mail.ru
269. *Savintsev Yuri Petrovich*, IGM SB RAS, savincev1940@mail.ru
270. *Sayfulin Marsel Zhaudatovich*, ISSP RAS, sayfulinmarsel@yandex.ru
271. *Selivonin Igor*, JIHT RAS, inock691@ya.ru
272. *Serebriakov Denis Glebovich*, JIHT RAS, denser96@yandex.ru
273. *Seredkin Nikolay Nikolaevich*, JIHT RAS, nikser12@yandex.ru
274. *Sergeev Igor Nikolaevich*, KBSU, pirlfix@mail.ru
275. *Shadymov Vladimir Alexandrovich*, MIPT, vladimir.shadymov@gmail.com
276. *Shakhray Denis Vladimirovich*, IPCP RAS, +7(496)5221756, shakhray@icp.ac.ru
277. *Shapiyeva Aigerim Yerlanovna*, MIPT, +7(701)6043018, shapieva.ae@phystech.edu
278. *Shcherbakov Viacheslav Vladimirovich*, JIHT RAS, uncle.slavik@gmail.com
279. *Shemakhin Aleksandr*, KFU, shemakhin@gmail.com
280. *Shemanin Valery Gennadievich*, KubSTU NPI, vshemanin@mail.ru
281. *Sherstyuk Natalia Eduardovna*, RTU MIREA, nesherstuk@mail.ru
282. *Shestakovskaya Elena Sergeevna*, SUSU, leshest@list.ru
283. *Shevchenko Alexander Leonidovich*, JIHT RAS,

+7(495)4851044, shev@ihed.ras.ru

284. *Shikalov Vladislav Sergeevich*, ITAM SB RAS,
v.shikalov@gmail.com

285. *Shikin Valery Borisovich*, ISSP RAS, +7(496)5221098,
shikin@issp.ac.ru

286. *Shilkin Nikolay Sergeevich*, IPCP RAS, ushnur@ficp.ac.ru

287. *Shpatakovskaya Galina Vasilievna*, KIAM RAS,
shpagalya@yandex.ru

288. *Shpekin Michael Ivanovich*, KFU, MichaelS1@yandex.ru

289. *Shumikhin Aleksey Sergeevich*, JIHT RAS, +7(495)3625310,
shum_ac@mail.ru

290. *Shumilin Vladimir Petrovich*, MIPT, ushnur@ficp.ac.ru

291. *Shumova Valeria Valerievna*, JIHT RAS, +7(495)4842610,
shumova@ihed.ras.ru

292. *Shutikova Maria Igorevna*, MIPT, shutikova_maria@mail.ru

293. *Shutov Alexander Vladimirovich*, IPCP RAS,
shutov@ficp.ac.ru

294. *Shutov Grigoriy Maksimovich*, MIPT,
shutov.gm@phystech.edu

295. *Shvartsburg Alexander Borisovich*, JIHT RAS,
+7(495)4841810, alex-s-49@yandex.ru

296. *Sidorov Rodion Sergeevich*, CIAM, +7(495)3621381,
rodik@myrambler.ru

297. *Sidorov Vladimir Michailovich*, MIPT,
vladimir.sidorov@phystech.edu

298. *Sitnikov Dmitry Sergeevich*, JIHT RAS, +7(495)2294240,
Sitnik.ds@gmail.com

299. *Sitnikov Nikolay Nikolaevich*, SSC RF FSUE KRC,
sitnikov_nikolay@mail.ru

300. *Skorkin Vladimir Mikhailovich*, INR RAS, +7(499)1354043,
ckripovo33@yandex.ru

301. *Smirnov Evgeniy Borisovich*, FSUE RFNC–VNIITF,
ewgeny_smirnov@mail.ru

302. *Smirnov Nikolai Aleksandrovich*, FSUE RFNC–VNIITF,
+7(351)70635, deldavis@mail.ru

303. *Smirnov Vladimir Sergeevich*, JIHT RAS, smvl95@mail.ru

304. *Sofronitskiy Artem Olegovich*, KNRTU-KAI,
artempic8@mail.ru

305. *Sokolov Maxim Anatolievich*, FSUE RFNC–VNIITF,

sokolovm1982@mail.ru

306. *Sokolova Tatiana Sergeevna*, IEC SB RAS, +7(3952)511680, sokolovats@crust.irk.ru
307. *Son Eduard Evgenievich*, JIHT RAS, +7(495)4841655, utro-2007@mail.ru
308. *Sosikov Vasiliy Alexandrovich*, IPCP RAS, +7(496)5224125, vaso@icp.ac.ru
309. *Stankevich Aleksandr Vasilyevich*, FSUE RFNC–VNIITF, AlexVStankevich@mail.ru
310. *Starykh Elizaveta Dmitrievna*, Skoltech, yelizaveta.starykh@phystech.edu
311. *Stegailov Vladimir*, JIHT RAS, +7(495)4858545, stegailov@gmail.com
312. *Subbotin Dmitry Igorevich*, IEE RAS, subbotin1987@mail.ru
313. *Sultanov Valery*, IPCP RAS, sultan@ficp.ac.ru
314. *Sundeev Roman Vjacheslavovich*, RTU MIREA, +7(495)4330044, sundeev55@yandex.ru
315. *Sverdlov Aleksandr Viktorovich*, ITMOU, togg1@yandex.ru
316. *Svetlov Anton Sergeevich*, JIHT RAS, svetlov.anton.s@gmail.com
317. *Syrovatka Roman Alexandrovich*, JIHT RAS, syrovatkara@gmail.com
318. *Sytchev George Alexandrovich*, JIHT RAS, +7(495)4857981, george.sytchev@gmail.com
319. *Taer Mikhail Sergeevich*, KBSU, mavar2014@yandex.ru
320. *Taibinov Nikolay Petrovich*, FSUE RFNC–VNIITF, +7(35146)54841, taibinov2@mail.ru
321. *Ten Konstantin Alekseevich*, LIH SB RAS, kten276@gmail.com
322. *Torchinski Vladimir Moiseevich*, JIHT RAS, torchvm@yandex.ru
323. *Torunov Sergey Ivanovich*, IPCP RAS, +7(496)5224125, storunov@yandex.ru
324. *Triaskin Jaroslav Vladimirovich*, SPbSU, ubik33@yandex.ru
325. *Trifanov Ilya Vladislavovich*, JIHT RAS, trifanovpgt@gmail.com
326. *Trigger Sergey Alexandrovich*, JIHT RAS, +7(495)3625310, satron@mail.ru
327. *Tsirlina Elena Arkadievna*, JIHT RAS, elena2509@yandex.ru

328. *Tsventoukh Mikhail Mikhailovich*, LPI RAS, elley@list.ru
329. *Tsvetkov Mikhail Yurievich*, FSRC CP RAS,
     mtsvet52@mail.ru
330. *Turkin Vitaly Nikolaevich*, VNIIA(L), vturkin@vniia.net
331. *Umarov Iskander Rashidovich*, JIHT RAS,
     iskan1997@yandex.ru
332. *Ushakov Nikita Andreevich*, INR RAS,
     nikitaushakoff@gmail.com
333. *Ushnurtsev Andrey Evgenyevich*, IPCP RAS,
     ushnur@ficp.ac.ru
334. *Usik Aleksandr Yurevich*, IMP UB RAS, +7(343)3783779,
     alexandr-usik1990@rambler.ru
335. *Ustyuzhanin Evgeny Evgenyevich*, NRU MPEI,
     evgust@gmail.com
336. *Uvarov Sergey Vitalievich*, ICMM UB RAS, +7(342)2378312,
     usv@icmm.ru
337. *Vagner Sergey Aleksandrovich*, IPCP RAS,
     vagnerserge@gmail.com
338. *Vasilyak Leonid Mikhailovich*, JIHT RAS, +7(495)4841810,
     vasilyak@yandex.ru
339. *Veiko Vadim Pavlovich*, ITMOU, +7(812)2333406,
     vadim.veiko@mail.ru
340. *Verbanov Ivan Sergeevich*, CIAM, isverbanov@ciam.ru
341. *Vetchinin Sergey Petrovich*, JIHT RAS, +7(495)4841810,
     lab852@ihed.ras.ru
342. *Veysman Mikhail Efimovich*, JIHT RAS, bme@ihed.ras.ru
343. *Vidyuk Tomila Maksimovna*, ITAM SB RAS,
     vidyuk@itam.nsc.ru
344. *Vikhrov Evgeny Vladimirovich*, JIHT RAS,
     vikhrov.e@gmail.com
345. *Vilkhivskaya Olga*, SRC RF TRINITI, vilkhiv@triniti.ru
346. *Vilshanskaya Evgeniya Vladimirovna*, JIHT RAS,
     eva.villi@gmail.com
347. *Vladimirov Vladimir Ivanovich*, JIHT RAS, +7(495)4842429,
     syrovatkara@gmail.com
348. *Vlasov Aleksandr Nikolaevich*, RSREU, vlasov.a.n@rsreu.ru
349. *Volodin Lev Yurievich*, BMSTU, volodinlu@yandex.ru
350. *Volosnikov Dmitriy Vladimirovich*, ITP UB RAS,
     dima_volosnikov@mail.ru

351. *Vorobieva Galina Yurevna*, IPCP RAS, vorobeva@icp.ac.ru
352. *Vorobyev Akim Vladimirovich*, FSUE RFNC–VNIITF, vbrf@list.ru
353. *Vorobyova Marina Anatol'yevna*, FSUE RFNC–VNIITF, arykounov@gmail.com
354. *Vorontsov Alexander Gennadevich*, SUSU, vorontsovag@susu.ru
355. *Yakunin Alexander Konstantinovich*, FSUE RFNC–VNIITF, yakunin_aleks@mail.ru
356. *Yakushin Roman Vladimirovich*, MUCTR, yakushinrv@yandex.ru
357. *Yatsenko Pavel Ivanovich*, JIHT RAS, pavelyatcenko@yandex.ru
358. *Yusupov Damir Il'dusovich*, JIHT RAS, yusupovdi@ihed.ras.ru
359. *Zaikin Sergey Vladimirovich*, CIAM, svzaikin@ciam.ru
360. *Zakharov Stepan*, JIHT RAS, stepan.zakharov@phystech.edu
361. *Zaporozhets Yury Borisovich*, IPCP RAS, +7(496)5221474, yubz@icp.ac.ru
362. *Zelener Boris Borisovich*, JIHT RAS, bobozel@mail.ru
363. *Ziborov Vadim Serafimovich*, JIHT RAS, ziborov.vs@yandex.ru
364. *Zubareva Alla Nikolaevna*, IPCP RAS, +7(496)5224125, zan@ficp.ac.ru

AUTHOR INDEX