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This book consists of the abstracts of plenary, oral and poster contributions to the XXXII International Conference on Interaction of Intense Energy Fluxes with Matter (March 1–6, 2017, Elbrus, Kabardino-Balkaria, Russia). The reports deal with the contemporary investigations in the field of physics of extreme states of matter. The conference topics are as follows: interaction of intense laser, x-ray and microwave radiation, powerful ion and electron beams with matter; techniques of intense energy fluxes generation; experimental methods of diagnostics of ultrafast processes; shock waves, detonation and combustion physics; equations of state and constitutive equations for matter at high pressures and temperatures; low-temperature plasma physics; physical issues of power engineering and technology aspects.

The conference is supported by the Russian Academy of Sciences and the Russian Foundation for Basic Research (grant No. 17-02-20033).

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1. Power Interaction with Matter

Chemical elements under extreme conditions

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Behavior of chemical elements under extreme conditions is considered. Recent results of experimental and theoretical studies of matter at high energy densities are reviewed.

Accelerators for high energy density physics

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A new collaboration to prepare the high energy density physics program at FAIR–Facility for Antiproton and Ion Research has recently been established. We will report on recent experimental and theoretical activities of this collaboration and we will review the basic concepts of high energy density physics with intense heavy ion beams as a tool to induce extreme states of matter. The development of this field connects intimately to the advances of accelerator physics and technology and aims to investigate the properties of intense heavy ion beams as a driver for inertial fusion energy. We will cover the generation of intense heavy ion beams starting from the ion source and follow the acceleration process

and transport to the target. Intensity limitations and potential solutions to overcome these limitations are discussed. The current experimental activities on HIHEX, LAPLAS and PRIOR experiments will be reported. This research was supported by Bundesministerium für Bildung und Forschung grants 05P12RDFN6, 05P12RDB7, 05P12RDBK, 05P12RDRBN and 05K10RD, German Science Foundation–Russian Foundation of Basic Research, Russian grant of scientific school NSh-5814.2014.2, and National Natural Science Foundation of China grants (U1532263, 11505248, 11375034, 11205225, 11275241, and 11275238).

Advanced methods of electron acceleration to high energies

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The report presents an overview of the rapidly developing research in many laboratories of the world, aimed at creating a new generation of accelerators of relativistic electrons. Electron acceleration to ultrahigh energies of teraelectronvolt range and the creation of compact sources of relativistic electrons and hard x-rays requires the development of new methods of acceleration of electrons with an acceleration rate is much greater than achievable with traditional radio-frequency accelerators. Among these methods, the most actively developing approaches are based on the use of wake fields generated in plasma by intense beams of charged particles (electrons or ions) or by relativistic-intense femtosecond laser pulses. Progress in laser-plasma acceleration of electrons to energies of a few GeV [1] opens up the possibility of an experimental study of a multi-step acceleration to high energies with the use of a new generation of multipetawatt class power lasers and determines the relevance of theoretical analysis of the optimal parameters of laser-plasma accelerator systems [2, 3]. The report also discusses recent results on different mechanisms of high-energy electrons generation [4, 5] required for many applications.

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[4] Andreev N E, Pugachev L P, Povarnitsyn M E and Levashov P R 2016 *Laser Part. Beams* **34** 115–122
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Laser interferometer gravitational wave observatory: Machine review and contribution of the Institute of Applied Physics RAS

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Only two years after T Maiman's discovery in 1960 of the first laser M E Gertsenshtein and V I Pustovoit proposed to use Michelson interferometer for detecting gravitational waves. They noted the main advantages of such detectors—wide band and high sensitivity—compared to solid state receivers that are massive cooled cylinders where natural acoustic oscillations are excited under the action of gravitational waves. The authors also pointed that correlation processing of measurements of two and more detectors is required.
A laser interferometer gravitational wave observatory (LIGO) was originally proposed as a means of detecting these gravitational waves in the 1980s by R Weiss, K Thorne and R Drever. Study of the noise and performance of such detectors and further concepts to improve them led to proposals for long-baseline broadband laser interferometers with the potential for significantly increased sensitivity. One of the key ideas that allowed the researchers to challenge the then (and even now) fantastic detector sensitivity was to use a high finesse Fabry–Pérot interferometer inside each arm of the Michelson interferometer. This trick multiply increasing effective arm length

was employed two more times: making use of the so-called power recycling mirror and signal recycling mirror.
The LIGO detectors observed gravitational waves from the merger of two stellar-mass black holes. Those observations demonstrated the existence of binary stellar-mass black hole systems. That was the first direct detection of gravitational waves and the first observation of a binary black hole merger.

Noncontact laser microsurgery of 3D living objects for use in reproductive and regenerative medicine

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Laser microsurgery has enabled highly precise and delicate processing of living biological specimens. We present the results of using femtosecond (fs) laser pulses in assisted reproductive technologies. Femtosecond laser dissection of embryos' outer shells (so called laser-assisted hatching) as well as laser-mediated detachment of the desired amount of trophectoderm cells (so-called embryo biopsy) required for preimplantaion genetic diagnosis were successfully performed. The parameters of laser radiation were optimized so as to efficiently perform embryo biopsy and preserve the viability of the treated embryos. Effects of application of fs laser radiation in the infrared (1028 nm) and visible (514 nm) wavelength ranges were studied. We also applied laser microsurgery to develop a new simple reproducible model for studying repair and regeneration in vitro.

Nanosecond laser pulses were applied to perform localized microdissection of cells spheroids. After microdissection, the edges of the wound surface opened, the destruction of the initial spheroid structure was observed in the wound area, with surviving cells changing their shape into a round one. It was shown that the spheroid form partially restored in the first six hours with subsequent complete restoration within seven days due to remodelling of surviving cells.

Ablation of tantalum and vanadium: Strength of liquid phase under a single-pulse action of femtosecond laser

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Femtosecond laser interactions with metals are described by the two temperature model [1]. Rapid isochoric heating and nonequilibrium bulk melting of a surface layer on a picosecond timescale are accompanied by the development of cavitation processes in the melt rarefaction wave and ablation of some melt in the form of a thin spall plate in a condensed state [2]. Ablation of tantalum has a bright specificity due to its high mechanical strength and low thermal conductivity. In this paper we study the ablation spall of tantalum and vanadium. An interferometric method is realized using a frequency-modulated pulse for diagnosing a dynamics of fast deformations with a spatial and temporal resolution under the action of a single laser pulse. Using an interferometric continuous monitoring technique [3], we have investigated the motion of the surface of a tantalum and vanadium targets in the case of femtosecond laser ablation near the threshold at picosecond time delays relative to the instant of laser exposure. The tensile strength of heated metals in a condensed state has been determined experimentally at an expansion rate of $\sim 10^9$ s^{-1}.

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Features of radiation of d-metals (gold) in the nonequilibrium electrons and lattice heating by femtosecond laser pulses

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Theoretical analysis of the spectrum of the thermal radiation of gold in terms of electron heating to temperatures above 10^4 K and for lattice temperature above 10^3 K in the relaxation period of electrons and lattice temperature was conducted, suggesting that long-range order of the crystal structure was not yet destroyed. It was shown that changes in the nature of the thermal radiation of gold will be determined mainly by interband radiative recombination of electron-induced smearing of the conduction electrons at high electron temperature, as well as the change in frequency of the electron–phonon collisions due to a significant heating of the lattice.

Creation of the wear resistance NiCrBSi coatings by laser cladding and subsequent deformation processing

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NiCrBSi coatings obtained by gas powder laser cladding are characterized by significant undulation and roughness. In present work the possibilities of using surface deformation processing (frictional treatment by sliding indenters carried out at various technological parameters) for ensuring a high-quality surface and additional increasing micromechanical and tribological properties of the surface layers of NiCrBSi laser clad coatings are considered. Furthermore the frictional treatment forms the favorable compressing residual stresses on the surface of NiCrBSi coatings. Frictional treatment leads to deformational dissolution of strengthening phases in solid solution resulting in lattice parameter growth. The very dispersed gradient layer is in evidence on the finished surfaces. This work was done with financial support of the Russian Foundation for Basic Research, grant No. 16-38-00452, within the complex program of the Ural Branch RAS, project No. 15-9-12-45.

The development of heterogeneous materials based on Ni and B_4C powders using a cold spray and stratified selective laser melting technologies

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The work is devoted to the development of scientific and methodological bases of production fundamentally new functionally graded heterogeneous materials based on ceramic B_4C powders with various concentrations in the initial mixture (30, 50, 70% by weight) and ductile metal metal Ni binder using additive technologies—combined method of cold gas-dynamic spraying (cold spray), followed by selective laser melting. It is shown, there is the dependency of the microstructure of track according to size of the ceramic particles in the range of 3–80 microns. It is observed, crushing (approximately in 2–3 times smaller initial particles) of ceramic particles occurs inside track as a result of exposure to laser radiation. The resulting tracks show growth microhardness up to 1000 MPa, B_4C with increasing concentration in the starting mixture.

Determination of thermo-mechanical ablation thresholds to sodium chloride irradiated by short laser pulses

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For the study of thermo-mechanical ablation thresholds ionic crystals was conducted the research of optical damage to sodium chloride by ultrashort laser pulses with duration $\tau = 40 \pm 2$ fs [1]. This pulse duration shorter than the other τ, used in similar experiments [2]. It was found, that the energy density of the threshold of the optical damage of the sodium chloride surface by laser pulses with a duration of 40 ± 2 fs was $E_{\rm cr} = 94 \pm 2$ MV/cm.

In case of damage to the sodium chloride surface laser irradiation ($\lambda = 800$ nm, $\tau = 40$ fs) for a surface densities of the power $I = 24$–90 TW/cm^2, calculation gives the ablation pressure 2.4–13.0 mbar. Previously in [3] it was specied, that for $\tau = 40$ fs it should be expected that $E_{\rm cr} = 100 \pm 5$ MV/cm (relative error of measurement $\epsilon_1 = 5\%$). In the case of $\tau = 40 \pm 2$ fs, will $\epsilon_2 = 5\%$. Then, according to [4], for $E_{\rm cr}$ ($\tau = 40 \pm 2$ fs) obtain ambiguous value $\epsilon = (\epsilon_1^2 + \epsilon_2^2)^{1/2} = 7\%$, and have a value $E_{\rm cr} = 100 \pm 7$ MV/cm.

The experiments that were carried out showed good coincidence with predicted values.

This work was supported in the framework of the base part of the Russian DES government task KBSU for years 2017–2019, project No. 3.8382.2017.

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Ultrafast destruction of quartz optical fibers

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An experimental study of the process of ultrafast destruction of the optical fibers, representing the links, is carried out. Under the influence of the laser radiation the destruction zone of quartz optical fibers (the plasma zone) occurs and spreads towards the radiation [1]. The main attention was directed to the registration of destruction when detonation-like mode of the propagation. In the experiments, we have used experimental quartz optical fibers in CNS RAS and industrial fibers connection. The stored fibers after passing of "optical detonation" have been investigated by scanning electron microscope. It was found that the destruction of the core and shell of quartz fibers has a multilevel nature from micro to nanosize. A numerical analysis of the possible hydrodynamic mode of the propagation of the plasma zone in the framework of the approximation of a continuous medium is carried out [2].

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The influence of the SiO_2 barrier layer on the glass composites laser ablation studies

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The influence of SiO_2 barrier layer on the laser ablation destruction threshold energy values of the glass composites with two components oxide films of TiO_2–Me_xO_y composition studies in the continuing [1–3] works have been fulfilled. The alloying Me_xO_y oxide amount was about 2 or 10 mass %. The oxides summary mass content in the film-forming sol was about 5 mass %. A substrate was the M0 type float-glass. The films were drown on the sample at the speed of 3.8 mm/s from the sol.
The film thickness, its refractive index and the film reflection coefficient values have been measured by the spectrum ellipsometer, light transmission in visible range and microhardness experimentally measured too. The composites laser ablation destruction under the irradiation of the pulse laser radiation with time duration of 20 nanoseconds or 300 microseconds was studied by the procedure given in [1, 3]. The threshold energy density dependences on the film thickness and its microhardness values are similar so it is necessary to consider the losses of the laser radiation energy due to the reflection at the films surface.

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The temperature field in laser ablation of a target at low temperatures

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After work [1] were performed computational experiments on laser ablation. We studied temperature field of the target in "subthreshold" approximation. The moments' method was used to solve heat equation. The decision was simplified for small values of some parameters: $l \ll 1$ and $T_s \ll T_a$ (l is typical size of the target's heating area, T_s is surface temperature, T_a is typical ablation temperature). The adequacy of the results assessed in comparison with the works of other authors and from general principles [2,3]. The solution has the form

$$\dot{T}(t,T,l) = \frac{\alpha\kappa(I_s l - \kappa T)}{2c\rho\kappa l}, \qquad \dot{l}(t,l) = \frac{\alpha\kappa(\alpha l + 1)}{c\rho\alpha l},$$

where $T = T_s - T_0$ is exceeding the target temperature T_s above its initial value T_0, κ, c, ρ are thermal conductivity, heat capacity and density of the target and I_s is the intensity of the absorbed laser radiation on the front of the laser ablation. This system of equations adequately describes the dynamics of the temperature field in the target material in the initial stages of the laser ablative destruction, when the temperature of target's surface is much smaller than the critical value.

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The investigation of the stirosil low-molecular polymer dissipation process different impurities under the continuous laser radiation

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During the investigation the principles of the stirosil low-molecular polymer dissipation with different impurities under the continuous laser radiation exposure were studied. The ytterbium laser LK-1000-OM with the operating wavelength of 1.07 μm and the output up to 1 kW was used as the radiation source. The experimental facility layout and the technique of experiments are given in the paper. The data of the sample mass loss during the exposure and the material dissipation depth at the conclusion of the exposure were obtained from the experiments. The calculated model of the studied polymer dissipation under the continuous laser radiation was worked out. It is found thatthe deviation of the calculated data from the experimental ones is less than 4% for the computation of the sample mass loss and 10% for the computation of the dissipation depth. According to the experimental results the rate of the mass loss per unit of area versus the power density of the incident laser radiation relationship was determined. The parameters of laser radiation such that the carbon residue loss starts were defined. Obtained results can be used for the polymer parameter optimization.

Ablation of metal heated through transparent media

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Action of ultrashort (subps, ps) laser pulse through transparent liquid onto absorbing metal is considered. We use one dimensional two-temperature (2T) hydrodynamics and molecular dynamics to follow evolution of contact boundary separating metal and transparent liquid. Five subsequent studies described are as follows: (i) two-temperature stage lasting few ps; (ii) decay of pressure "jump" between liquid and metal. The decay sharply accelerates contact and produces a shock in liquid and a rarefaction wave in metal; (iii) creation of a heat affected zone (HAZ) during the 2T stage; (iv) multiple nucleation in rather thick zone inside the HAZ and in the tail of rarefaction due to stretching and weakening of cohesive bonds as a result of heating; (v) deceleration of the spallation plate (SP) by inertia of liquid. Thus, on the one hand, the SP is decelerated by displaced liquid volume and on the other hand, the SP is pushed ahead by the flow of the pieces of expanded foam coming to SP from its back (relative to the contact) side.
Histories of pressure, temperature and other parameters are presented.
Work is supported by the Russian Foundation for Basic Research, grant No. 16-08-01181, and the Presidium RAS, program "Thermophysics of high energy densities".

Irradiation of thin metal film standing without support by femtosecond laser in the case when illuminated spot is small

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Two-temperature combined thermal and mechanical problems (lasting few picoseconds) are considered in the case of a thin film together with late evolution up to nanoseconds time scale. Thin here means that the film is thinner than a heat affected zone. Previously the cases of films deposited onto substrate have been studied in full 3D geometry. The case of unsupported films has been considered previously but only when size of the illuminated spot was large. Thus one-dimensional approach was applicable. The 3D problem of finite size with aspect ratio of the order of 10 is much more complicated. Solution of this problem will be presented. Work is supported by grant from the Russian Foundation for Basic Research No. 16-08-01181 and program of the Presidium RAS "Thermophysics of high energy densities".

Separation of film from substrate by radially polarized laser beam

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We consider structures produced by tightly focused radially polarized femtosecond laser pulse. The structures are produced at the targets composed from thin film on dielectric substrate. Work is supported by the Russian Foundation for Basic Research (grant No. 16-08-01181) and program of the Presidium RAS "Thermophysics of high energy densities".

Ablation dynamics of film–substrate targets when thickness of film is more than thickness of heat affected zone

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We consider ablation dynamics in the case when film thickness d_f is larger than thickness d_T of a heat affected zone (HAZ). This problem is difficult relative to the problem when $d_f < d_T$. Film is heated supersonicaly up to the contact with substrate if $d_f < d_T$. Then pressure rise at a contact accelerates a motionless matter of a film in the direction out from substrate. If $d_f > d_T$, then a shock go out of a HAZ. Shock moves matter of a film in opposite direction, in direction to substrate. Shocks refracts on a contact.

Situation depends on is spallation plate (its thickness is comparable with d_T) separated or not. Work is supported by the Russian Foundation for Basic Research (grant No. 16-08-01181) and program of the Presidium RAS "Thermophysics of high energy densities".

Expansion of multilayer target heated by short pulse with large penetration depth

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Problem of heating of a multilayer structure by hard x-ray laser is considered. Particular structure studied is made up from alternating metallic films m1–m2–m1–m2–..., each of 50 nm thick, deposited onto a thick Si or SiO_2 substrate; here m1 and m2 are metal one and metal two. It is supposed that an attenuation depth $d_{\rm att}$ in m1 amd m2 metals for the x-ray laser frequency is much larger than total thickness of the multilayer x-sandwich. In the substrate the attenuation depth is order of magnitude larger than in metals. Duration of pulse is short, much shorter than electron–ion temperature relaxation. An electron–ion temperature relaxation coefficient α (called coupling parameter) is different for metals m1 and m2. Thermal conduction coefficients κ are approximately the same $\kappa_1 \sim \kappa_2$ for both metals. The depth $d_{\rm att}$ is shorter for metal m2 where the coupling parameter is weaker. We consider a two-temperature stage where energy is absorbed mostly in m2; during and after absorption, the energy is conducted thermally to m1 where coupling is stronger. In this situation ion subsystem in m1 is heated faster than in m2. We compare pressure rise and beginning of expansion of the system. Work is supported by grant from the Russian Foundation for Basic Research No. 16-08-01181 and program of the Presidium RAS "Thermophysics of high energy densities".

Interaction between ultrashort laser radiation and metal surface: Influence of multidimensional geometry to the formation of surface nanostructures

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Nanostructuring of the surface of irradiated metal is one of the most important effects caused by laser pulses exposure. Mechanisms of formation of nanostructures are very complex and there's a lot to be unknown. Extreme scenarios are the following: on the one hand, the interference of the incident electromagnetic wave and surface plasmons and on the other hand, the non-uniform ablation of the surface, i.e. hydrodynamic movement and (or) separation of substances. In case of resonance with plasmons the greatest importance has the factor of electromagnetic interference. In the other case of ablation thermal physics, hydrodynamics and phase transitions play the first role. Non-uniform ablation along the surface of the irradiated target is considered in the paper. In both cases in consideration non-uniformity is caused either by heterogenity of periodic modulation of the laser intensity along the surface of the target volume or by the finite size of the laser spot irradiating the thin film on the substrate. For the analysis of these cases the popular one-dimensional two-temperature model [1] is for the first timeexpanded to two-dimensional (2D) geometry.

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Formation of foamed structure in aluminum and iron melts at high-rate tension

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Under the influence of ultra-short laser or electron irradiation, the isochorically-heated metal melts and expands, due to the pressure gradients at first and due to inertia thereafter. The ablation of molten metal within the energy deposition area goes similar to the spall fracture in solids. Both the complete fracture of melt on droplets and the melt solidification as a foamed structure at some intermediate stage of tension are of practical interest.

We investigate by means of molecular dynamics the regularities of the foamed metal melts formation at the high-rate tension. Melt fracture includes several stages [5]: growth of large and collapse of small pores; destruction of walls between pores with formation of jets; fragmentation of jets on droplets. The foamed melt retains till the void volume fraction exceeds 0.9 at least. The foamed structure evolution is controlled by surface tension. Via the dimensional consideration, we propose analytical estimations for the time evolution of the mean radius, pressure in the system and the work on melt tension. The void size grows in time even after termination of further melt extension, while the pore number decreases due to collapse of smallest ones. Simulation of the foamed melt cooling down to room temperature shows an amorphous foamed metal structure formation, which persists over time.

This work was supported by the grant from the President of the Russian Federation (project No. MK-9111.2016.8) in the part of the foamed structure formation, and by the grant from the Russian Science Foundation (project No. 14-11-00538) in the part of the investigation of the melt tensile strength.

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Dynamics of a cavity in metal melt: Molecular dynamics and continuum simulations

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The first part of this work is devoted to check the applicability of the Rayleigh–Plesset equation [1] for description of dynamics of a spherical cavity in metal melt. Molecular dynamics (MD) simulation was used for this purpose. Aluminum melt was chosen. Cases of pure collapse and pure growth of a cavity were investigated. Melt temperatures 1000, 1500, 2000 K and strain rates 10^8, 10^9, 10^{10} s^{-1} were considered. The program Lammps [2] with the interatomic potential [3] for aluminum was used for the MD simulation. Continuum simulation was carried out by the Euler method with a time step of 0.001 ps. Good agreement of continuum and MD simulations was obtained. The second part of this work is devoted to the study of interaction between two cavities in the aluminum melt at its full tension with the true strain rate $\dot{\varepsilon} = 3 \times 10^9$ s^{-1} at temperature 1000 K. A qualitative description of different variants of interaction is presented. The obtained results can help to understand the mechanism of interaction of cavities that occurs due to cavitation at high rate tension of the melt.

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Numerical analysis of nanoparticles formation during femtosecond laser ablation of aluminum

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Nanoparticles of different sizes and colloid mixtures of them are widely used in science and technology. Femtosecond laser ablation is an effective way to produce particles of different sizes. In order to generate the particles more effectively, it is necessary to understand the mechanisms underlying laser ablation.

We use a continuum-atomistic model based on approach [1] for simulation of laser ablation, in which molecular dynamics is used for description of the atomic subsystem while the electronic one is described by the energy conservation equation solving. The main advantage of the combined model in comparison with hydrodynamic approaches is the accurate representation of fragmentation of a metal both in solid and liquid phases on small time and space scales. In our model the laser radiation absorption is calculated according to the Helmholtz equation. For description of permittivity, electron thermal conductivity and electron-ion coupling we apply wide-range models [2] which makes it possible to simulate double and multiple laser pulses.

We investigate the structure of the ablation plume, the mechanisms of nanoparticles formation and the size distribution of them.

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The atomistic simulation of the core-shell nanoparticle formation

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The study of core-shell nano-objects is of a great interest [2], because core-shell particles, which consist of a noble metal, and a dielectric or semiconductor, exhibit an optical resonance in the visible range [2], where the resonance frequency depends on the geometrical parameters of the particles. Gold-silicon particles can be formed by laser ablation by irradiating multilayer films with the ultrashort laser pulses. It is necessary to understand the mechanisms of their formation to synthesize the particles with specified characteristics. In this work the processes occurring during the formation of gold-silicon core-shell particles were examined.

At the initial stage various models of potential gold-silicon interactions were tested and the values important for the modeling of the formation of the particles were estimated. Also the comparison of experimental data on the melting temperature and surface tension were produced for pure components with the results obtained for different models. Then a cooling of a gold-silicon system was simulated. It was shown that liquid Au–Si alloy amorphized in subsurface at cooling rates greater than 1 K/ps, and crystallized at lower cooling rates. Distribution of the components tends to be inhomogenious during crystallization (Si and Au-enriched regions appeared).

The processes of the core-shell particle formation were simulated. It was found that crystalline silicon melts when contacting liquid gold at the temperature below silicon melting point. If liquid gold contacts liquid silicon then the melt becomes homogeneous in a few picoseconds. Also the liquidus curve were estimated from the molecular dynamic simulation and compared to experimental data.

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Finite-difference time-domain simulation of the interaction between ultrashort laser pulses and metal nanoparticles

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Metal nanoparticles (NPs) serve as important tools for many modern technologies [1]. However, the proper microscopic models of the interaction between ultrashort laser pulses and metal NPs are currently not very well developed in many cases. One part of the problem is the description of the warm dense matter that is formed in NPs after intense irradiation (e.g. see [2]). Another part of the problem is the description of the electromagnetic waves around NPs. Description of wave propagation requires the solution of Maxwell's equations and the finite-difference time-domain (FDTD) method is the classic approach for solving them. There are many commercial and free implementations of FDTD, including the open source software that supports GPU acceleration [3,4]. In this report we present the results on the FDTD calculations for different cases of the interaction between ultrashort laser pulses and metal nanoparticles. Following our previous results [5], we analyze the efficiency of the GPU acceleration of the FDTD algorithm.

The study has been funded by the Russian Academic Excellence Project "5-100".

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Wide-range model of Ag response on femtosecond laser irradiation

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We present a model of femtosecond laser interaction with Ag bulk targets. The model takes into account laser-induced excitation of electron subsystem, electron-phonon coupling, electron heat conduction and hydrodynamic motion of matter. Using the model, we perform simulation of matter response in regimes similar to that observed in pump-probe experiments.

On the emittance growth under non-symmetric laser-plasma coupling conditions

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Emittance characterizes angular and transverse spread of a particle beam. For practical purpose it should be as low as possible. We report calculations of the emittance of electron bunches, accelerated in wakefields behind laser pulses propagating in guiding structures: capillary waveguides and plasma channels. The calculations are done using the model consisting of equations of motion for electrons, equations for angular harmonics of wakefields and expressions for angular and radial harmonics of laser fields in guiding structures [1, 2]. We had shown, that the condition of conservation of low energy spread and low normalized emittance (about few mm mrad) of

accelerated electron beam impose about an order of magnitude more severe restrictions on the accuracy of laser power focusing into a guiding structure (plasma channel or capillary waveguide), than the requirements of obtaining high energy gain, low energy spread and low losses of accelerated particles, studied earlier [1–3]. Particularly, the angle between the axis of guiding structure and the axis of laser pulse propagation should not exceed 0.1 mrad, and the transverse displacement of the laser radiation focusing point from the guiding structure axis should not exceed 0.5% of the characteristic inner radius of the guiding structure.

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Electrons accelerating backward in the interaction of femtosecond laser pulses with solids

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We study the interaction of femtosecond laser pulses with solid targets. Calculations on interaction of petawatt laser PHELIX GSI, Darmstadt, Germany and solid aluminum targets with preplasma with two different profiles corresponding to two different contrasts of the laser pulse incident normally at the the target. Density profiles have been previously obtained by two-temperature hydrodynamic modeling. Then calculations were performed of the interaction of the laser pulse with PHELIX parameters and of the laser pulse duration is 10 times shorter and with the layer of the overcritical plasma

density. The simulations were performed to analyze the existing theoretical concepts on the interaction of relativistic femtosecond intense laser radiation with the sharp boundary overcritical density at different pulse durations. In addition, modeling is produced of the interaction of laser pulses with parameters of the facility at the Helmholtz Institute in Jena, Germany incident at an angle of 45 degrees with a p-polarization at the second harmonic on the solid target with the sharp density profile. Results are compared with the experiment. In all cases with sharp density profile except the electrons traveling forward inside the target, which are well described in the literature, we observed high energy electrons traveling back from the target. With the help of the test particle trajectories the mechanism of acceleration back from the target is analyzed.

Injection and acceleration of electrons in the plasma wake field generated by short laser pulse

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Wake plasma waves which induced by high-intensity laser pulses are of interest as a way to achieve high energies of electrons. In particular, the creation of sources of high-energy electrons for injection into a laser-plasma accelerator was studied in [1,2]. The goal of this work is development of methods of electron acceleration in plasma which is exposed to the low energy(40 mJ) femtosecond laser pulse. The laser pulse energy and the plasma density distribution was selected in accordance with the experiment [2]. Calculations were performed using the three-dimensional "particle-in-cell" method [3] with the following parameters: the length of the laser pulse at half maximum is equal to 15 μm, the beam radius at the level $1/e^2$ is equal to $r = 8.4$ μm, the maximum intensity at the focus equal to

9.4×10^{17} W/cm^2. The density distribution of hydrogen plasma is Gaussian, with $n_{\max} = 6.6 \times 10^{19}$ cm^{-3}.
For the laser pulse power in excess of critical one for relativistic self-focusing, the pulse undergo self-contraction with steepening of the pulse front. These processes lead to the self-modulational instability, generation of the wakefield plasma wave, injection and acceleration of electrons. The maximum energy of accelerated electrons approaches ~ 8 MeV, that agrees with the experimental data [2].

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The structure of wake fields excited in plasma by different drivers

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Research of new acceleration methods of electrons in the plasma wake fields is being widely conducted with usage of various sources (drivers) of relativistic nonlinear waves in plasma. The paper presents the comparative characteristics of the fields structure in the wake wave, excited in the plasma by three different drivers: by the laser pulse or short proton and electron bunches. The ability of wake wave to capture externally injected electrons, as well as different injection techniques for each driver are studied on the basis of the obtained structure of accelerating and focusing fields in the wave.

Generation of short electron bunches by a laser pulse crossing a sharp boundary of plasma

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The process of the generation of a short electron bunches by a laser pulse of relativistic intensity that passes through a sharp boundary of plasma and their subsequent acceleration in the wake wave of a laser pulse has been analytically studied [1, 2]. It is shown in one-dimensional geometry that a physical mechanism that is responsible for the generation of electron bunches is self-injection of electrons into the wake field of a laser pulse, which occurs due to the mixing of electrons during the action of the laser pulse on plasma. The length of the trapped electron bunch is determined by the effect of kinematic grouping, which consists in the fact that electron self-injection into the wake wave occurs at the point of space and the moment of time when the previously trapped electrons are close to this point. Subsequently, during acceleration of trapped electrons in the wake wave, the length of the bunch increases as a result of the initial spread in the conditions of electron injection and their mutual repulsion in the bunch. Simple analytic relationships were obtained that can be used for estimating the length, charge of an electron bunch and the spread of electron energies.

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Spin dynamics of electrons emitting synchrotron radiation during laser plasma acceleration

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In this work the process of multistage laser wakefield acceleration of polarized electron beams is considered. Electrons are accelerated under the action of fields generated by the laser pulse in the parabolic plasma channel. During acceleration relativistic electrons undergo betatron oscillations and emit synchrotron radiation, which affects beam characteristics. To describe this process the relativistic equation for the electron motion in electromagnetic fields with the radiative reaction force in Landau–Lifshitz form was used [1] and quantum recoil effects were taken into account [2].

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Trajectory control of small rotating projectiles by laser discharges

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The experimental and theoretical analysis of the trajectory control of small rotating projectiles by laser discharges has been performed. The laser spark was generated by 1.06 μm Nd-YAG laser (3 J, 5 ns

pulse duration). It was shown that the spark generates a strong shock wave, a hot gas spot, and a slow air jet. The gas heating is considered as a primary mechanism for the pressure redistribution along the projectile surface and the trajectory change.

Three series of experiments were done in a supersonic wind tunnel with a rotating projectile. We demonstrate the rotating projectile's destabilization by a single laser spark and 3-pulse laser bursts. The pulse separation in the burst was varied from 50 to 100 μs. In all three cases the projectile destabilization has been demonstrated.

A theoretical analysis of the interaction of an oblique shock wave with a hot spot was made. An analytical criterion for a strong interaction between a shock wave and a hot layer has been found. It was shown that the critical temperature of the hot layer increases with the shock wave angle decrease relative to the flow direction, and decreases with the Max number of the shock wave. Thus, for a flat shock wave ($\alpha = 90^\circ$) at M = 3 the critical temperature in the hot layer is $T'/T = 1.8$. For an oblique shock ($\alpha = 40^\circ$) the strong interaction regime requires $T'/T = 6.5$. The numerical modeling demonstrates an excellent agreement with the theoretical predictions. The energy required for the projectile's trajectory deviation by $\alpha = 1^\circ$ is determined by the critical overheating of the gas layer, the minimal length of the interaction and the critical diameter of the hot spot. The estimations show the critical energy for the gas heating about 2 mJ/10 of the trajectory change for the length of interaction ~ 3.5 cm.

Diagnostic of plasmas created in relativistic laser matter interaction at high laser contrast

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Studying the parameters characterizing extremely non-Maxwellian, transient plasma states created in relativistic short pulse laser–matter interaction, remains at the forefront of advancing the scientific understanding of highly complex plasma phenomena. In this work we present an experimental evidence of a highly ionized plasma state with a solid electron density obtained due to interaction of the high contrast 50 fs relativistic laser pulse with Ti-foils. Intensity of the second harmonic (400 nm) Ti-sapphire laser pulse onto the target reached 10^{19} W/cm^2. Complex diagnostic set-up was used for measuring a characteristic plasma radiation, a bremsstrahlung radiation provides by suprathermal electrons and an energy distribution of energetic electrons escaped the target. Results of measurements have been used to characterize parameters of plasma created in short relativistic laser–matter interaction at high laser contrast.

Laser-driven magneto-inertial fusion with magnetized hohlraum

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The external magnetic field parallel to the hohlraum axis of symmetry is an important technical issue, including penetration of laser radiation into a plasma and confinement of charged particles, used in the laser-driven magneto-inertial fusion. The external magnetic field on the final stage of compression contributes to the excitation in plasma electromagnetic helicon waves, whose energy can penetrate into the plasma and absorbed throughout the plasma volume. We consider the problem that can be represented as two related subtasks: powerful broadband radiation interaction with the central or axial-symmetric magnetized target; the interaction of intense laser radiation with the inner walls of the hohlraum and dense high-temperature plasma. It is assumed that hohlraum is used for implosion of magnetized plasma target, as a source of broadband x-rays, formed by an external laser system. It is obvious, in this case the plasma dynamics equations and the laser radiation transfer equation, as the boundary and initial conditions are preserved. The system of equations describing the processes of heating and evaporation of the metal wall of the hohlraum under the influence of thermal radiation from the plasma volume with the radiation flux density, which takes into account the incident laser beam on the wall, is presented. Such system doesn't take into account the hydrodynamic processes in condensed matter, and consists of the heat equation in a moving (associated with the evaporation wave front) coordinate system with an axis perpendicular to the evaporation surface. Thermal processes occurring on the hohlraum walls are described.

About laser shocks dynamics for complex spot and structured targets

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We have analyzed the laser inducted shock behavior in experiments with double focal spot, in particular, the cumulative effect in double layer foam-metal targets (which is explained by the multiple collisions of individual shocks in the structured target) [1]. Two focal spots were obtained by the laser beam splitting. A photographic objective has been employed to image the target rear face onto a streak. In order modeling the experiment with a 2D hydrodynamic simulations [2], we assumed an axial-symmetric approximation (double-rings spatial profile for the laser spot). Some results of experimental shock dynamics are in a good accordance with the theoretical and numerical predictions, but others demand for new models. The reasons are discussed in the report. A A is grateful to STSM visit grant in the framework of COST Action MP1208 "Developing the physics and the scientific community for inertial fusion" for support.

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Hydrodynamic model of interaction of laser radiation with deuterium–tritium target

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In this work, the hydrodynamic model of two-temperature plasma in conditions of inertial fusion is considered. The system of hydrodynamic equations with the counts of kinetic phenomena (viscosity, thermal conductivity and the temperature difference between ions and electrons) the radiation transfer equation and beam of heavy ions are calculated. In the framework of the model based on the hydrodynamic system, the results of several numerical experiments, the study of which is substantive interest, are considered: (i) shock wave propagation in spherical geometry for two temperature plasma; (ii) the impact of high-power laser pulse on a target, confining a mixture of deuterium and tritium; (iii) the impact of heavy ion beam at a hot dense plasma bunch. In the first problem important role play the electron conductivity and discrepancies between ions and electrons temperatures on the front of shock waves. In the second problem the compression of deuterium-tritium mixture due to the expansion of the outer shell is considered. An important role is played by the wave of electron thermal conductivity and the shock wave propagating inside the target. In the third problem the heating of dense hot plasma bunch by beam of heavy ions is considered. This research was funded under the target program No. 0115PK03029 "NU–Berkeley strategic initiative in warm dense matter, advanced materials and energy sources for 2014–2018" from the Ministry of Education and Science of the Republic of Kazakhstan.

Calculation of the ion stopping in a dense plasma by the Monte Carlo method

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The calculation of thermonuclear target parameters for heavy ion inertial fusion requires adequate quantitative description of processes of heavy ion interaction with a dense plasma in a wide range of parameters. Therefore, in order to know the properties of the dense plasma under different conditions, the most attractive way is a computer experiment, which provides answers to many important questions necessary for the use of inertial confinement fusion dense plasma at energy issues. In this paper, Monte Carlo method for simulation of ions trajectories in a dense plasma of inertial connement fusion is presented. The main advantage of the calculation by the Monte Carlo method is that it allows you to take into account any physical process directly. For example, local and non-local inelastic energy losses, bound energy between atoms replacing collision and so on. The calculation of characteristics of Ti, Fe, Xe ions beam in targets of H, D, T, D–T mixture, Be, Cu are carried out. The result of computer simulation are numerical data on the dynamic characteristics, such as energy loss, penetration depth, the eective range of the particles, stopping and straggling. Also, according to the results of the work was created program of the 3D visualization of the ion trajectories in a dense plasma of inertial connement fusion. This research was funded under the target program SRW No. 0115PK01011 “Development of informational-program package for modeling and visualization of dense plasma properties in inertial connement fusion for 2015–2017” from the Ministry of Education and Science of the Republic of Kazakhstan.

Features of primary radiation damage in Fe–Cr alloy near free surfaces

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Influence of interfaces on primary radiation damage in Fe–10Cr alloy was studied in the framework of molecular dynamics method. For this purpose simulation of atomic displacement cascade evolution near free surfaces with different crystallographic orientations was performed. For a description of the interatomic interaction in the alloy we used many-body potential, constructed according to the concentration-dependent embedded atom method [1]. Crystallographic indices of the irradiated surfaces were (110) and (111). The energy of the primary knock-on atom did not exceed 20 keV. Analysis of the simulation results showed that the number of survived point defects after generation of atomic displacement cascade near the free surface can be several times greater than the number of defects generated in the bulk sample by displacement cascade away from the interfaces. After the irradiation of the free surfaces the volume of the samples contained more vacancies than interstitial atoms. Calculations show that crystallographic orientation of irradiated free surface significantly affects the character of primary radiation damage of the material. Craters are formed on the (111) surface, while for the (110) surface formation of vacancy type dislocation loops takes place. It was found that the different character of surface damage is connected with anisotropy of motion of shock waves formed by atomic displacement cascades in the volume of the crystallite.

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Sensitivity of PbSnTe:In films to the radiation of free electron laser

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The band gap Eg of the $Pb_{1-x}Sn_xTe$ solid solution depends on the composition and temperature. Near the liquid helium temperature, the increase in the Sn content from $x = 0$ (PbTe) to $x \sim 0.35$ leads to a reduction of E_g from ~ 0.19 eV to zero, and for $x > 0.35 E_g$ increases again. Within $x \sim 0.24$–0.29 ($E_g \sim 0.04$–0.06 eV) adding to this compound of In leads to a "pinning" of the Fermi level in the forbidden zone. Thus the resistivity of narrow-gap semiconductor $Pb_{1-x}Sn_xTe$:In at $T = 4.2$ K becomes comparable to the resistivity of conventional insulators at $T \sim 300$ K. Giant value of the static permittivity of more than 2000 at $T = 4.2$ K is one of the reasons for the low ionization energy of impurity centers in $Pb_{1-x}Sn_xTe$:In, which corresponds to the submillimeter (terahertz) wavelength range. In addition, the features of $Pb_{1-x}Sn_xTe$ as a solid solution (i.e., a disordered system), lead to a complex spectrum of energy levels of impurity centers, the filling of which depends on the magnitudes of applied electric and magnetic fields or the lighting conditions in the region of fundamental absorption (far IR region). The paper presents analysis of experimental data on observation of photoresponse in $Pb_{1-x}Sn_xTe$:In, grown by the method of molecular beam epitaxy by exposing samples to the powerful radiation of the Novosibirsk free electron laser (wavelength range of about 70–240 μm) under the different measurement conditions.

The work is supported by the Russian Foundation for Basic Research, grant 17-02-00575.

Generation of terahertz radiation in the interaction of a laser pulse with clusters

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We have studied generation of terahertz radiation in the interaction of a femtosecond laser pulse with a spherical cluster. The problem of penetration of laser radiation into a cluster with a size smaller than the skin depth and laser wavelength in vacuum has been considered. It is shown that the laser field in the cluster plasma can increase substantially when the laser frequency is close to the frequency of the dipole or quadrupole mode of a spherical cluster. The angular, spectral, and energy characteristics of terahertz radiation are studied for the case of a laser pulse with a Gaussian time profile. Conditions are found at which terahertz waves are emitted mainly at angles of 45° and 135° with respect to the propagation direction of the laser pulse, which corresponds to the quadrupole directional pattern. The spectral and energy characteristics and the time profile of the terahertz signal are shown to depend substantially on the density of free electrons in the cluster. For an underdense cluster plasma, when the electron density is lower than critical, the radiation spectrum has a sharp peak at the frequency of the quadrupole eigenmode of a plasma sphere. As the electron density increases and becomes higher than critical, the spectral line at the frequency of the quadrupole mode vanishes and a broad bell-shaped maximum appears at the frequency comparable with the reciprocal of the laser pulse duration. The total energy of terahertz radiation is calculated, and its dependence on the density of free electrons is analyzed. It is shown that this energy as a function of the electron density has maxima when the laser frequency coincides with the frequencies of the dipole and quadrupole eigenmodes of a plasma sphere.

High-n hollow ion emission from Si ions pumped by ultraintense x-rays from relativistic laser plasma

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The first observation of high-n hollow ions (ions having no electrons in the K or L shells) produced in Si targets via pumping by ultraintense x-ray radiation produced in intense laser-plasma interactions is reported. The existence of these new types of hollow ions in solid density plasma has been found via the observation of highly resolved x-ray emission spectra of silicon ions from the front and rear side of the target. This has been conrmed by plasma kinetics calculations underscoring the ability of powerful radiation sources to fully strip electrons from the innermost shells. It has been demonstrated that Si plasma created by PW-power optical laser pulses reaches the radiation dominant kinetics regime.

Powerful x-ray radiation of a plasma generated during head-on collisions of high-energy plasma flows

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The conversion of plasma flows kinetic energy to photon energy during collisions is one of possible ways to generate vacuum-ultraviolet and soft x-ray radiation. The possibility of such conversion was theoretically predicted in [1, 2]. Experimental research results of the pulse soft (0.1–1 keV) x-ray source with total energy yield up to 50 kJ are shown. The radiation pulse was generated during a head-on collision of two low-temperature plasma flows immersed in a longitudinal magnetic field. The plasma flows with the velocities up to 4×10^7 cm/s and total energy up to 200 kJ are formed by a coaxial accelerator operating in pulse gas puffing regime. Diagnostics of the high-temperature plasma formed by plasma flows collisions was carried out by comparing the observed intensities of the spectral lines with the results of detailed kinetic calculations made in the stationary approximation. The electron temperature for the plasma containing nitrogen ions is about 130–140 eV. The electron density obtained by interferometry measurements varied from 10^{16} to 10^{17} cm^{-3}. This work was financially supported by the State Corporation "Rosatom" (state contract No. N.4h.44.9B.16.1011 of 29 February 2016).

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Ultra-bright x-ray source generation from thin Al and Fe solid foils irradiated with 200 TW fs laser pulses

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Observation of hollow ions in x-ray spectra have been proposed as an indirect approach to determinate ultra intense x-ray in strongly non-uniform plasmas. X-ray emission from thin Al and Fe foils irradiated by femtosecond laser pulses was investigated at the sets of experiment at J-KAREN facility, Ti:Sapphire hybrid laser system Kansai Photon Science institute of Quantum Beam Science Research Directorate. For spectroscopic measurements, high spatial resolution x-ray spectrometers equipped by spherically bent mica crystals were implemented. Our measurements and corresponding simulations by ATOMIC code confirm that laser pulses with intensity $I \sim 10^{21}$ W/cm^2 are able to generate ultra-bright x-ray source with $I \sim 10^{18}$ W/cm^2 irradiating targets with $Z = 13$ but this x-ray intensity is insufficiently to excite hollow atoms transition for solids with $Z = 26$.

Focal spot imaging of terahertz subpicosecond pulse by THz field-indiced optical second harmonic generation

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Optical imaging of spatial distribution of electric field in the focal spot of the terahertz pulse was developed. The technique is based on the THz electric field-induced second harmonic generation in the nonlinear centrosymmetric crystal ($SrTiO_3$). The measurements of the spatial distribution of focal spot of terahertz radiation with the electric field strength over 1 MV/cm were conducted.

Experimental investigation of the soft x-ray spectra of laser produced plasmas on the facility "Kanal-2"

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The report presents an experimental investigation of the soft x-ray spectra of laser produced plasmas on the facility "Kanal-2", which based on a nanosecond laser with a large number of transverse modes (≈ 1000) and wide spectrum (≈ 2.6 nm). Materials Be, B_4C, C_2H_4 and Cu were used as targets, pulse duration was 2.5 ns and the power density on the targets was about 10^{13} W/cm^2. The spectra

of soft x-rays were obtained by grazing incidence spectrograph (GIS-S), and the emphasis was placed at the ranges for "water window" (2.34–4.38 nm) and "carbon window" (4.4–5 nm). It was found that the B_4C can be used as an effective source of radiation at these ranges.

The work was partially supported by Russian Foundation for Basic Research, grant 16-02-00293.

X-rays diagnostics of the hot electrons distribution in the intense laser interaction with metal targets

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We have developed models of characteristic and bremsstrahlung x-rays generation by laser produced relativistic electrons propagating in a metal target. The models take into consideration energy losses of the electrons, cross-sections of the x-rays generation, an absorption of the x-rays and target thickness. Developed models has allowed us to analyze results of measurements of K_α and bremsstrahlung x-rays from silver targets irradiated by laser pulses with intensity about 2×10^{19} W/cm^2. Modelling of measurements of bremsstrahlung x-rays from a bulk silver target by the filters and the knife methods revealed two-temperature hot electrons distribution with lower temperature about 110–140 keV and higher temperature in the wide range of 0.6–1.7 MeV described by the well-known scalings. The ratio of the energies contained in the components with the higher and the lower temperatures is about 10–14%. Modelling of the K_α x-rays yield from the bulk target and a silver foil of 10 μm

thickness, deposited on a plexiglass substrate, showed that the recirculation of hot electrons in the foil can be neglected, and the conversion efficiency of the laser energy into the energy of hot electrons is less than 2%. A possibility to analyze parameters of the hotter electron component taking into account errors of the measurements is under discussion.
Theoretical part of the work was supported by grant No. 14-50-00124 from the Russian Science Foundation.

Microfocus source of intense x-ray radiation

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Microfocus x-ray tubes are comparatively new means for extraction of unique information on micro and macrostructure of materials. Limit of the power dissipating on a standard planar anode of the tube is about 10 W under diameter of the excitatory electron beam spot about 100 μm.
This paper has suggested a tube generating continuous x-ray high intensity flux diverging from a small area. X-rays are formed in a channel executable in the form of a funnel in the thick anode. Conical flare of the funnel operates for reflection and direction of the hollow electron flow spreading along the symmetry axis into a cylindrical part of the funnel at a big angle in relation to the axis. X-rays are generated within the process of a cascade of reflections and absorptions of electrons by walls of the funnel cylindrical stage and brought outside through the cylindrical channel basis hermetically sealed by a foil made of metal having a low atomic number. The idea of multiple rise of radiation intensity consists in increase of the surface area from which the emission of x-rays originates using an anode with a funnel-shaped channel in comparison with a planar through-target anode. Effective area of radiation (bringing-out) of quantum in the suggested variant is determined by the area of the

cylindrical channel basis and, in principle, it can be arbitrarily small. It is related with the fact that x-ray radiation spreading not in the direction of the external basis of the cylindrical channel is absorbed by walls of the thick anode. Value of the power dissipating on an anode can achieve 300 W and more.
The design of the tube was produced with utilization of the author's CAE FOCUS (http://www.focuspro-soft.com). The research has been supported by grant No. 15-19-00132 from the Russian Science Foundation.

X-ray photoelectron spectroscopy studies of the crystalline samples after laser exposure

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The aim of work was to study the impact of ultrashort laser pulses on the surface of the crystalline samples [1, 2]. The surface of NaCl crystals and other ionic compounds was examined outside and in the crater of thermo-mechanical ablation using an x-ray photoelectron spectrometer (XPS). Methods of work were described previously [3]. An important parameter, which can be found using XPS, is the binding energy in atoms. The measured binding energy (E_m) determines the value of the maximum line components. We compared E_m with a reference value of the binding energy (E_r) outside and in the crater. Also relative shear of lines studied, calculated according to the formula: $\eta = (E_m - E_r)/E_m$. It was found that the measured values of the binding energy exceed the reference values, i.e. $\eta \neq 0$. It can be seen, that the studied atoms and molecules are able to the tangible interact on the crystalline material surface. The results of the work the effect of significant impact was found on the surface and the binding energy of crystalline samples of high-intensity ultrashort laser pulses.

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Spatial configuration of fast ion source created in femtosecond laser plasma of cluster targets studied by ion pinhole imaging method

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A plasma induced by high-intensity femtosecond laser is considered for a long time as versatile compact source of fast ion beams for micromachining, precision microsurgery, proton radiography of ultrafast plasma phenomena, etc. In this context, the use of gas cluster targets provides a set of definite advantages such as the absence of debris and wide-angle ion emission. However, the spatial configuration of the ion source formed in fs laser-cluster target interaction has not been studied well yet. Ion pin hole imaging method is proposed and applied for the first time to study the processes of fast ion acceleration in the interaction of 10^{17}–10^{18} W/cm^2 35 fs laser pulses

with CO_2 cluster target. It was obtained the region with highest fast ion yield is spatially separated from that one with peaked yield of x-rays. This fact is most likely associated with the destruction of clusters by laser prepulse at the best laser focus. This assumption is consistent with time-resolved optical shadowgraphy data showing the formation of the plasma channel in the vicinity of the best laser focus prior the arrival of the main laser pulse. The anisotropy in the ion source spatial configuration was examined for for different laser focusing position inside the gas cluster cloud.

X-ray radiography measurements of short-lived hydrodynamic phenomena in astrophysically relevant plasma flows

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For studying astrophysical phenomena, experimental research related to laboratory astrophysics using an intense laser was performed. In the experiment with 1.5 ns, 600 J laser pulses focused to 300 μm focal spot at solid laminate target in presence of 20 T poloidal magnetic field the dynamics of the plasma outflows were studied by means of pulsed x-ray radiography.
Pulsed x-ray radiography allows the study of fast evolving phenomena like shock compression of matter or plasma outflows, interactions with gas or plasma atmosphere reducing smearing of even high velocity phenomena ($v > 100$ km/s) to the μm scale. Using a thin 20 μm wire for diagnostics it was demonstrated successfully reproducible high-quality x-ray radiography in a new configuration of

x-ray source and detector. Spatial resolution better than 20 μm has been achieved at magnification $M = 17.8$. The data indicates a better signal to background ratio using frequency double laser light, although the difference is not important for the quality of the radiography. A question of detailed measurement of the spectral composition of the radiation recorded by the detector was analyzed as well. Finally, an example on a laboratory astrophysics experiment demonstrated the high resolution obtained with this configuration.

Numerical simulation of proton-radiography experiments at Geant4

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The high-energy proton radiography in the investigations of dense dynamic target provides greater penetration depth, spatial resolution, density resolution and dynamic range than conventional x-ray methods. The new proton microscopy facility with beam energy of 247 MeV is developing for investigation of static and dynamic objects with areal density of 5 g/cm^2. The facility is designed according to the scheme of proton microscope [1] with increasing an image of objects. In this work, using Monte-Carlo Geant4 code, was developed the virtual model of proton-radiography facility, which is includes quadrupole lenses, vacuum detector, target chamber, collimator and source of primary protons. Primary calculation of ion optics of facility was performed by COSY Infinity code. In frame of development of virtual model were written programs, which are allows calculation of phase characteristics and angular distribution of beam. The full-scale numerical simulation of proton-radiography experiments with static objects (Cu, Plexiglas step wedges) and static models of dynamic process, in investigation of anomalous compressibility of docosane and shock-compression of Xe gas, were performed

with the model. Developed model can be used for numerical simulation of proton-radiography experiments at PRIOR facility at FAIR project.

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Method for reconstruction of volume density distribution in dynamic targets from their proton radiography images

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Using proton microscopy facilities PUMA [1] at ITEP and PRIOR [2] at GSI, series of experimental investigation of extreme states of matter in dynamic processes were performed. An important task in such experiments is to restore volume density distribution in the target from a single proton radiography image. Recurrence algorithm of inverse Able transform was implemented in Matlab to solve this problem. During the tests it was found that the algorithm is very sensitive to distortions in the original data. In this regard a number of distortion compensating techniques were implemented. Noise suppression effected by multilevel wavelet thresholding and an exponential averaging filter. To compensate blur of images Lucy–Richardson deconvolution algorithm applied. Fitting of beam intensity profile by asymmetric Gauss function is used to compensate instability of proton beam. Demonstration of developed tools was performed with results of underwater electrical wire explosion experiments at PRIOR facility at GSI and investigation of detonation of TNT at PUMA facility at ITEP. Additionally, results of abnormal compression in docosane experiment at future 247 MeV facility, which is modeled in Geant 4, were processed.

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The gravitational-optical method for recognition between the galaxies and antigalaxies in the universe

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A gravitational-optical distinction between the cosmic galactic and antigalactic clusters in the Universe is proposed. It is based on the totally gravitationally neutral universe (TGNU) concept proposed earlier (see e.g. [1]). The TGN-universe concept includes (a) enlarged (unbroken baryon, CPT and full $\pm M_{\rm gr}$ gravitational) symmetries between massive fermions of ordinary matter (OM)–ordinary antimatter (OAM), as well as between dark matter (DM)–dark antimatter (DAM) particles and (b) the opposite gravitational properties of all massive and massless bosons, including OM-photons–OAM-antiphotons etc. The composite (OM+DM)-galactic and (OAM+DAM)-antigalactic clusters are equally presented and mutually gravitationally repulsive in TGNU. The cosmic OM- and OAM-photons, emitted by far-remote galaxies and antigalaxies (both visible but purely optically indistinguishable), get basic gravitational differences in the TGNU-concept. The OM-photons must be gravitationally attracted to the (OM+DM)-clusters and gravitationally repelled by the (OAM+DAM)-clusters and the OAM-photons, on the contrary, must be gravitationally attracted to the (OAM+DAM)-clusters and repelled by the (OM+DM)-clusters. The far-remote (OM+DM) galactic and (OAM+DAM) antigalactic clusters are optically-gravitationally distinguishable and detectable, because their OM- and OAM-photonic rays deviations will be opposite if we observe them near a massive (OM+DM) deviation-galaxy or a star from our galactic group, which moves fast enough on the heavenly sphere across direction to these far-remote clusters.

Simulation of nonlinear waves interaction on the boundary of dielectric liquid with finite depth in a strong tangential electric field

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Nonlinear dynamics of the free surface of finite depth nonconducting fluid with high dielectric constant under the action of strong tangential electric field is investigated in the present work. The equations of boundary motion admit exact solution in the form of nonlinear localized waves of arbitrary shape propagating without distortion along the surface of liquid in the direction of (or against the direction of) the external field. Despite the fact that the nonlinear waves can separately propagate without distortion, the interaction of counter-propagating waves can result in deformation of the boundary. Numerical modeling methods based on using of dynamic conformal transforms of the region occupied by the fluid into parametric strip of auxiliary variables were chosen for the study of interaction of the oppositely traveling waves. The simulations show that nonlinear waves are actually deformed in result of their collisions; herewith the effect of nonlinearity is inversely proportional to the liquid depth, i.e. deformation increases with depth decreasing.
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Criteria for disintegration of an uncharged conducting liquid jet in a transverse electric field

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An uncharged cylindrical jet placed between a pair of flat electrodes is considered. In the trivial case, when the electric field is absent, the only possible equilibrium configuration corresponds to the jet with circular cross-section. In the presence of a potential difference between the electrodes, the jet is deformed by the electrostatic forces: its cross-section stretches along the electric field lines. In the case of the mutual compensation of the electrostatic and capillary forces, a new equilibrium configuration of the jet can appear [1]. In a sufficiently strong field, the balance of the forces becomes impossible, and the jet splits into two separate jets. In the present work, we find the range of the parameters (the applied potential difference and the interelectrode distance), where the problem of finding the equilibrium configurations of the jet has solutions. Also we obtain the conditions under which the solutions do not exist and, consequently, the jet splits. The results are compared with the previously studied limiting case of infinite interelectrode distance [2].
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Pre-breakdown hydrodynamic characteristics of weakly conductive liquid media in the high nonuniform electrical field

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A quasi-exponential formula for the current–voltage characteristics of low conductive dielectric fluids in the presence of high-voltage electric field was obtained analytically by solving the system of equations [1]. These equations are for the pre-breakdown charge formation in quasi-neutral media such as transformer oil and they were derived earlier by the first author of this work. The high-voltage electric field is created by the "wire on plane" system of electrodes. A linear dependence of the radius of the micro-breakdown zone in the vicinity of the edge of the needle electrode was obtained from this system of equations.
The MacCormack method was used for numerical analysis of the pre-breakdown characteristics of weakly conductive liquid media. The problem was solved taking into account the influence of the space charge field on the field of high-voltage electrode system "wire on plane". The results are presented for several values of the applied dc voltage.

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Atomic mechanisms of grain structure restructuring in surface of aluminum during ion implantation

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The study of the features of structural transformations in the surface layer of nanostructured aluminum at various modes of ion implantation was carried out. Molecular dynamics simulation was used for investigation of structure changes in irradiated crystallites. Interatomic interaction potential for aluminum was described in the framework of the embedded atom method. Used potential allowed describing with high accuracy many mechanical and physical properties which are very important for the simulations of the high-energy loading. Aluminum atoms were used as the incident particles. Velocity of incident atoms was directed normal to the free surface. Its value varied from 200 to 2000 Å/ps. It is shown that high energy loading resulted in the change of the number, size and shape of the grains. The role of mechanical preloading of simulated samples was revealed.

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"Point-like" neutron source based on high-current electron cyclotron resonance ion source with powerful millimeter wave plasma heating

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Neutron tomography is one of the most exciting recent achievements of nuclear physics. It opens up opportunities for a wide range of various microscopic studies of physical, chemical and biological objects. It is of note that neutron tomography requires dedicated neutron source, i.e. paraxial source with low angle spread. The only sources now able to deliver required neutron beams with sufficient intensity are nuclear reactors and large-scale accelerators in pair with collimators. The use of point-like neutron sources based on laser plasma induced by focusing of powerful femtosecond laser radiation onto a neutron-producing target was proposed lately. The isotropic neutron flux from a point-like source with small angular spread (determined by the source size) seems to be useful for neutron tomography. High resolution comparable to one obtained with collimated neutron beams may be derived from the source of small size. A possibility of compact powerful point-like neutron source creation based on a high current electron cyclotron resonance ion source with gyrotron plasma heating is discussed. The fusion takes place while bombardment of deuterium (or tritium) loaded target by high-current (1 A) focused (the size of the ion spot on the target is the size neutron source, smaller than 100 μm) deuterium ion beam with energy of 100 keV. The yield of the source based on deuterium–deuterium reaction is estimated on the level of 10^{11} s^{-1} (10^{13} s^{-1} for deuterium–tritium reaction).

Modelling of electron–ion relaxation in ion tracks in AlN and SiC

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Swift heavy ion (SHI) irradiation of materials initiates the formation of non-equilibrium near-solid density plasma (so called warm dense matter—WDM) along the SHI path with high-temperature electrons (excited by the inelastic interactions with SHI) and cold ion lattice (e.g. ee [1]). Non-equilibrium WDM is a very complicated object for theoretical description; processes of electron-electron and electron-ion relaxation in such systems on the fs-timescale are still poorly understood.

Here we present the results of WPMD-based calculations for the initial 100 fs stage of relaxation in a SHI track region in wide-bandgap semiconductors AlN and SiC. Using eFF potential [2] we investigate the aspects of SHI's energy deposition in material and describe such processes as material ionization, electron–electron relaxation and subsequent energy transfer into the ion subsystem. eFF is based on a simplified solution to the time-dependent Schrödinger equation. It performs explicit dynamics of electrons (represented as gaussian wave-packets) and can be considered as more advanced alternative to the traditional thermal-spike method and two-temperature molecular dynamics.

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Thermal radiation of drops which are formed in metal foils heating by heavy ion beam

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We consider irradiation of a thin metallic foil heated by an intense heavy ion beam under the assumption that the energy deposition is volumetrically uniform. The non-stationary behavior of a foil is described by 1D-equations of gas dynamics in mass coordinates. The system of equations is governed by equation of states. It is supposed that the main contribution to thermal radiation is made by drops of metastable vapor–droplet medium which is formed at adiabatic expansion of the foil heated by heavy ions. The method for definition of dependence of complex index of liquid metals refraction on temperature and radiation wavelength from available experimental data is offered. The Lorenz–Mie theory is used for calculation of absorption and dispersion sections of drops. Nucleus number evolution is described by analogy with gases kinetic theory. In the result we have infinite system of ordinary different equations. Using of continuous function of nucleus size distribution leads to Fokker–Plank equation. The system of ordinary different equations and Fokker–Plank equation are solved by numerical methods. Using of implicit finite-difference schemes allows reaching of quasi-stationary nucleation regimes. The absorption and the scattering coefficients at each point of vapor–droplet medium is defined by integrating on drops radii. Influence of the droplet formation onto interpretation of the experimentally measured brightness temperature is considered for thin lead foil volumetrically heated by 450 MeV/u uranium ion beam having duration 50 ns.

The influence of the electric field near the insulator in the plasma focus chamber on neutron yield

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The work describes a plasma focus (PF) device based on the capacity energy storage. The plasma focus is a source of neutron radiation. When operated using deuterium as a working gas, 2.5 MeV neutrons are emitted. In the case of using mixture of deuterium and tritium 14 MeV neutrons are emitted. This work presents the results of research the influence of the electric field in the PF chamber on neutron yield. It is shown that the increase in intensity electric field of the electrode gap next to the insulator contributes to the formation of a homogeneous current plasma sheath. Developed and tested the PF chamber with a modified design of the cathode: at the cathode surface has a groove of triangular cross section, located on a circle whose center is on the axis of the PF chamber. Use of triangular section grooves on the cathode increases the neutron yield in PF chambers several times.

Microwave synthesis of nanoselenium in polymeric surfactant systems

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Nanoselenium materials have a great scope of applications nowadays. Amorphous red nanoselenium attracts attention because recently it were discovered its wonderful properties in mammals life. It is known elemental selenium has a great significance as nutrient and can be used in different forms as nutritional supplement. Moreover, selenium has anticancer properties and can act as antioxidant. It has potential applications in pharmacology, medicine for diagnostics, therapeutics and toxicology as antidote in the case of heavy metals toxication. The main problem of selenium applications in medicine as drug and dietary supplement is its toxic properties. Sometimes this fact may restrict its applications. But nanoselenium gives good opportunity to overcome this obstacle because of reduced toxicity as compared with inorganic and organic compounds of selenium. We have studied new ways of synthesis of nanoselenium in biocompatible form with the use of microwave radiation. A number of biofriendly surfactants was used. As polymeric media polyvinyl alcohol and polyvinylpirrolidone were used in their water solutions. Nanoselenium samples were synthesized in microwave reactor; here the mixture of water solutions of polymer, surfactant, selenious acid, sulphur dioxide was treated. Nanocomposites received were investigated. Uv-viz, Raman spectroscopy, x-ray, electronic and optical microscopy were used. Conclusions on the mechanism of stabilization of nanoparticles were made.

The influence of microwave radiation on the solid-phase recovery process of ilmenite concentrate

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In recent years increasing interest among researchers is paid to the use of microwave heating in the processing and enrichment of metal ores. Advantages of microwave processing materials include penetrating radiation, controlled distribution of high-frequency electric field, selective influence on the material and increase of the speed of the solid-state reaction. A preliminary evaluation of economic efficiency in carbothermic recovery of metals from oxides showed that under optimal conditions the recovery process will significantly reduce energy consumption compared to traditional methods.
Study of the effect of microwave radiation on the process of solid-phase recovery of ilmenite concentrate carried out in high temperature microwave brand M-01 with the frequency of the radiation 2450 MHz and power 800 W. The ore-coal briquettes was placed in a ceramic crucible and recovered at a temperature of 1000 °C during a specified time interval. The radiation power density during the experiment was 2.5 MW/m^2. Evaluation of the phase composition and degree of recovery of ilmenite concentrate was performed using x-ray diffractometer Shimadzu XRD-7000. Visualization of the products of the recovery was carried out using scanning electron microscope S-3400N Japanese firm Hitachi. In the work evaluated the influence of microwave radiation on the degree of recovery of ilmenite concentrate and phase composition of the reaction product. It is shown that microwave impact greatly accelerates the process of recovery of metallic iron in the ilmenite concentrate, allows to reduce the temperature of the process by 1.5–1.8 times and to increase the degree of recovery by 50% compared to traditional high temperature methods.

Band structure and transparency of the two-dimensional photonic crystal with a central defect

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Polycapillary optics technologies are developing in x-ray optical systems laboratory of KBSC RAS [1]. High quality of our polycapillary fibers produced by stretching and femtosecond laser allow us to investigate optical effects occurring in 2D photonic crystals. We present the new method for calculating electromagnetic fields distribution in polycapillaries with central hollow defect. The method is similar to that used for the calculation of the band structure of the crystal lattice with defects. Numerical calculations of polycapillary fiber transparency and intensity patterns at the exit surface have been compared with experimental data.

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Thermalization of laser excited metal nanoparticles: Wave packet molecular dynamics

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In recent times, nanoparticle (NP) interaction with ultrashort laser pulses has been a subject of significant interest. Among the most interesting questions is the possibility to obtain plasma with near-solid density (warm dense matter) by use of ultrashort laser pulses of TW/cm^2 fluences. As non-equilibrium warm dense matter is a very complicated object for a theoretical description in this work we use *ab initio* molecular dynamics to investigate relaxation processes in Al NPs. Unlike density-functional theory or classical methods, wave packet molecular dynamics provides a unique possibility to describe non-adiabatic effects and at the same time is not very computationally demanding. We apply the eFF potential in our study to Al nanocluster after an intense laser excitation. In this method electrons are represented as floating Gaussians and interactions between electrons are restricted to pairwise components only. In recent study [1] this method has been successfully used to study the response Al NP on irradiation by short laser pulses. In this report we present a further investigation of thermalization processes in laser excited aluminum NPs.

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Atomistic simulation of impurities segregation on the (0001) surface of the crystal α-Al_2O_3

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The information about the change of free energy of impurity in its transfer from the crystal bulk into the gas phase through the surface is significant to create the theoretical foundations of the high-temperature vacuum α-Al_2O_3 purification technology [1]. Free energy profile determines both the rate of impurities diffusion to the surface with subsequent sublimation and thermodynamic limit of purification relative to the different chemical elements. For this reason, the difference between the free energies between the surface and bulk states was calculated for a large set of two-, three-, and tetravalent impurities on the most stable surface (0001).

It was found that for trivalent ions with a radius close to that of Al, such as Cr and Fe, segregation energy is close to zero. This indicates a lack of pronounced segregation effect, which is consistent with the high solubility of these elements in corundum [2, 3]. With further increase in the size of the ions, G is decreased and segregation of impurities becomes energetically favorable. For sufficiently large impurities, such as Y, calculations predict a strongly pronounced segregation on the crystalline surface and slight solubility in bulk alumina which is confirmed experimentally [3].

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

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The influence of carbon surface topography on the kinetics of the oxygen reduction reaction

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Li-air batteries arouse particular interest due to their expected very high energy density of about 1700 $\mathrm{W\,h\,kg^{-1}}$ against 170 $\mathrm{W\,h\,kg^{-1}}$ for widely used Li-ion batteries [1, 2]. However, there are several obstacles to the creation of prototypes with such a high performance. In particular, the contribution of the cathode surface topography on the kinetics of heterogeneous processes in such systems remains insufficiently known.

In this work molecular dynamic simulation was used in order to investigate the influence of the carbon surface topography on the cathode–solvent interface structure near the following model cathodes: graphene plane, single- and multi-layer graphene edges. It was found that the topography of the carbon surface qualitatively influences the cathode–solvent interface structure and, as a result, the distribution of the main reactants (Li^+ and O_2) of the oxygen reduction reaction [1]. In comparison with the carbon plane, the topography of the graphene edge shows the accelerated adsorption kinetics and higher concentration of the oxygen. This can explain the increased formation of the reaction products at graphene edges after discharge of the Li-air batteries, observed in the experiments.

The calculations were run on the supercomputers MVS-100K and MVS-10P of the Joint Supercomputer Center of the Russian Academy of Sciences. The work was supported by grant from the Russian Scientific Fund (project No. 14-50-00124).

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The influence of surface charge and Au crystallographic faces on the interfacial structure of the ionic liquid [BMIM][BF_4]

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Understanding the interfacial structure of ionic liquids is important from the practical point of view. Ionic liquids have a variety of applications, which are based on heterogeneous processes. Previously, the effect of the two-dimensional ordering of electrosorbed ions was observed experimentally on different surfaces, but the factors that determine this effect is not fully clarified. Therefore, in this work we investigated the influence of surface charge and crystallographic faces on the interfacial structure of ionic liquid by molecular dynamic simulation. 1-butyl-3-methylimidazolium tetrafluoroborate ([BMIM][BF_4]) is chosen as the ionic liquid and three types of Au surfaces are studied: (001), (111) and the artificial non-structured surface. The surface charge density varies in the range from -70 to 70 μC/cm^2. Concentration distributions of $[BMIM]^+$ and $[BF_4]^-$ were obtained. The simulation shows the influence of crystallographic faces on the two-dimensional anions ordering and their surface orientation. Square and triangular lattices are formed on the positively charged (001) and (111) surfaces, respectively. The lattice structure appears gradually with the surface charge increasing to 70 μC/cm^2. On the non-structured surface the long-range order of the ions $[BF4]^-$ is not observed. $[BF4]^-$ ions are oriented by two or three fluorine atoms to the (001) and (111) surfaces, respectively. Calculations were performed on the clusters MVS-100K and MVS-10P of JSCC RAS. This work was supported by the Russian Science Foundation (project No. 14-50-00124).

Molecular dynamics simulation of solvent impact on the association reaction of Li^+ and $[O_2]^-$ ions

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The impact of solvent on the reaction of Li^+ and $[O_2]^-$ ions association was studied by molecular dynamics simulation, which is important for the efficiency improvement of Li–air batteries. Three solvents (acetonitrile, 1.2-dimethoxyethane, dimethyl sulfoxide) with various donor numbers (DN = 14, 20 and 30 respectively) are used in the simulation. The potential of mean force for the reaction of ion association in each solvent was calculated. The simulation shows that activation energy of the reaction has the highest value in dimethyl sulfoxide. This fact correlates with the experimental works, which present that the reaction of ion association is better inhibited in high-donor-number solvents than in low-donor-number ones. All computations are carried out using the clusters of JSCC RAS (MVS-100K, MVS-10P). The work was supported by grant from the President of the Russian Federation No. MK-7873.2016.3.

Effect of high donor number solvent and electrode morphology on interfacial processes in Li–air batteries

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The work is focused on identifying the factors responsible for different electrochemical activity of carbon cathodes with different morphology in Li–air batteries. Molecular dynamics simulation was used for the interface structure investigation of the high donor number solvent dimethyl sulfoxide (DMSO) at the surface of carbon nanotube, graphene plane, single- and multi-layer graphene edge. It was determined that the solvent has the layered structure at the graphene plane, sidewall of the nanotube, and single-layer graphene edge. Moreover, the sharpness of the solvent layers decreases with increasing surface curvature. The multilayer graphene edge–solvent interface has qualitatively different chessboard structure. It was shown that an adsorption activation energy of O_2 molecules decreases in the order graphene plane, nanotube, graphene edge. Strong solvation of Li^+ in DMSO prevents ions adsorption, which is qualitatively different from our previous calculations for acetonitrile [1]. It can be concluded from these results, that nucleation and growth of products in DMSO is shifted from the surface towards the solvent bulk that, in turn, leads to capacity increase of Li–air batteries. This work was supported by grant from the President of the Russian Foundation, grant No. MK-7873.2016.3.

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Influence of carbon conductive additives on electrochemical double-layer supercapacitor parameters

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Electrochemical double-layer capacitors (EDLC) are emerging energy storage technology, highly demanded for rapid transition processes in transport and stationary applications [1], concerned with fast power fluctuations. Rough structure of activated carbon, widely used as electrode material [2] because of its high specific area, leads to poor electrode conductivity. Therefore there is the need for conductive additive to decrease internal resistance and to achieve high specific power and high specific energy. Usually carbon blacks are widely used as conductive additive.

In this paper electrodes with different conductive additives—two types of carbon blacks and single-walled carbon nanotubes—were prepared and characterized in organic electrolyte-based EDLC cells. Electrodes are based on original wood-derived activated carbon produced by potassium hydroxide high-temperature activation at the Joint Institute for High Temperatures RAS. Electrodes were prepared from slurry by cold-rolling. For electrode characterization cyclic voltammetry, impedance spectra analysis, equivalent series resistance measurements and galvanostatic charge–discharge were used.

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The plasma device at NRU MPEI for the high-heat plasma testing of refractory metals and inventing of new highly porous materials

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A device is constructed at the NRU MPEI for the investigation of high-temperature plasma-surface interaction and the high-heat plasma flux testing of refractory metals, used in fusion devices including the ITER. This device is a multi-cusp linear plasma confinement system. The magnetic system consists of coils, creating a longitudinal magnetic field up to 6 mT on the axis, and permanent magnet bars that form the magnetic cusps along the axis. Design parameters of stationary plasma discharge: current is up to 30 A, the density is up to 10^{18} m^{-3}, T_e is up to 4 eV with a hot fraction up to 30 eV, ion flux onto the test sample is up to 3×10^{21} $m^2 s^{-1}$, the working gas—He, Ar, D. Experiments are planned to develop a technology for highly porous structure of the surface of the refractory metal with a pore size and nanofibers of 50 nm. A novel scientific idea [1] of the growth of highly porous material layers under the high-heat plasma flux and the recent results of the first experimental observation of porous layers [2] will be used. This work was supported by grant No. 16-19-10531 from the Russian Science Foundation.

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Methods for reproduction of complex thermal and mechanical action of radiations and particles fluxes on barriers from constructional materials

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Need of development of methods for reproduction of complex thermal and mechanical action of radiations and particles fluxes (RPF) on a constructions of aircraft is proved [1,2]. Usually thermal action accompanies mechanical action. Constructions accumulate heat at repeated RPF actions. Such accumulation can reduce construction strength to mechanical RPF action and also to flight loadings.
Carrying out experimental studies for direct and repeated RPF influence localized on large-scale construction is impossible or expensive in many cases. As rule settlement and experimental approach [2] is used. Realization of this approach demands creation of devices set [3] for simultaneous modeling of thermal and mechanical RPF actions. Such set of devices is considered in present work.
Results of tests of fragments of composite multilayered constructions at reproduction of complex thermal and mechanical RPF action are given.

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Radiophysical properties of radiotransparent thermal protection materials in ablation mode

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Experimental method for assessing the impact of the effects of high-temperature ablation processes on the radio physical characteristics of radiotransparent thermal protection materials (RTPM) is developed. Researches for the following RTPM with various structures of glass fillers are completed: press material (RTP-200); glass-fiber laminate (GFR-CM); reinforced quartz material (HTRC-CM) and a thin-layer thermal protection coating (TCT). The influence of physicochemical transformations in the surface layer of RTPM on transmission and reflection coefficients of electromagnetic (EM) waves and on the value of their complex permittivity is determined. It is shown that changes of modulus of transmission coefficient after the high-temperature treatment make 1–2 dB of order of magnitude in the frequency range from 2 to 40 GHz for HTRC-CM, make 4 dB no more for GFR-CM, make 14 dB no more for RTP-200 and make 25 dB no more for TCT. It is worth noting that the most significant changes of transmission coefficient are observed in the short-wave region of EM spectrum. In the total the HTRC-CM has high-level operating reliability, whereas the radiophysical properties of RTP-200, GFR-CM and TCT deteriorate.

Artificially constructed plasmarons and plasmon–exciton molecules in two-dimensional metals

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Resonant optical excitation was used to create a macroscopic nonequilibrium ensemble of "dark" excitons with an unprecedented long lifetime in a two-dimensional electron system placed in a quantizing magnetic field. Exotic three-particle and four-particle states, plasmarons and plasmon-exciton molecules, coupled with the surrounding electrons through the collective plasma oscillations are engineered. Plasmarons and plasmon-exciton molecules are manifested as new features in the recombination spectra of nonequilibrium systems.

Radiation reaction effects of relativistic electrons in the strong field of an aligned crystal

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The influence of classical radiation reaction on the motion of the radiating charge itself has never been tested experimentally. It has been show recently [1] that classical radiation reaction effects, in particular those due to the near electromagnetic field, as predicted by the Landau–Lifshitz (LL) equation, can be measured in principle

using presently available facilities, in the energy emission spectrum of 30-GeV electrons crossing an aligned 0.55-mm thick diamond crystal in the axial channeling regime. The problem has previously been studied by the present authors [2–5].
In the present study we calculate the radiation damping of the transverse energy of the electrons channeled along the $\langle 110 \rangle$ axis of silicon and diamond crystals. In contrast with paper [1], we show that two terms in the Landau–Lifshitz equation are significant, whereas the authors of [1] take into account only the term proportional to the spatial non-uniformity of the external field strength.
The transverse energy change $\delta\epsilon(\omega)$ as a function of the emitted photon energy ω due to the radiation transition from the initial i to the final f state is $\delta\epsilon = \epsilon_f(E_i - \omega) - \epsilon_i(E_i)$, where E_i is the total initial electron energy. We present the correspondence of this quantum process to classical treatment based on the LL-equation.

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Producing of synthesis gas with predetermined H_2–CO ratio

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The two-stage pyrolytic technology, which consists of the biomass pyrolysis and the consequent high-temperature conversion of pyrolysis gases and vapours into synthesis gas by filtration through a porous carbon medium, allows to achieve both a high degree of biomass conversion into gaseous fuel and a high energy efficiency [1]. The ratio between the volume content of hydrogen and carbon monoxide in the produced synthesis gas depends on the elemental composition of the feedstock. For the main types of vegetable biomass this ratio is 1 : 1 within 20% [2]. This paper presents the

results of an experimental study of the effect of mode parameters of torrefaction (heating in oxygen-free environment and subsequent holding at a fixed temperature) on the elemental composition of the two types of vegetable biomass (wood and agricultural waste). Data on composition and volume of synthesis gas, calculated on the basis of measurements of the elemental composition of torrefied biomass, and analogous data, obtained at a laboratory installation as a result of two-stage pyrolytic conversion of torrefied biomass samples, showed good agreement. As it follows from obtained data, by using the two-stage pyrolytic conversion method as applied to the pre-torrefied biomass of different types it is possible to obtain a synthesis gas with a predetermined ratio of volume content of hydrogen to carbon monoxide in the range from 1 : 1 up to 2 : 1.

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Exothermic effect during torrefaction

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During biomass pyrolysis a decomposition of basic organic components (hemicellulose, cellulose, lignin), accompanying by exo- and endothermic effects, occurs [1]. These effects must be taken into account in the development of thermal methods of biomass processing, in particular torrefaction. Torrefaction is a low-temperature pyrolysis, carried out in a temperature range of 200–300 °C and used for improvement of biofuel consumer properties. There are presented the results of investigation of self-heating process, taking place during torrefaction. Experiments were performed at a laboratory installation simulating of column-type torrefaction reactor with indirect (through the wall) heating of processable raw material [2]. It was shown experimentally that at the temperature above 250 °C there is observed spontaneous biomass heating even when the

heater, providing heat supply through the wall, is switched off. As a result at the reactor axis the temperature exceeds the near-wall region temperature. Note that the amplitude of overheating increases along the reactor length. During heating of the pre-torrefied biomass self-heating in the temperature range 200–300 °C is not observed. This may be explained by the absence of hemicellulose and products of its thermal decomposition in torrefied biomass. The results of experiments at the laboratory installation are correlated with the results obtained during studying the thermal effects using the differential scanning calorimetry method. All the results can be used for modeling the thermal effects accompanying the wood biomass pyrolysis.

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Influence of heat treatment on the characteristics of solid fuels from agricultural waste

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In today's world one of the promising areas of energy development is using of biomass as fuel. Using of local energy resources in many cases in economic terms is more advantageous than imported fossil fuels. There is a problem of utilization of agricultural waste, which could be used as fuel. One of the most promising ways of fuel production from agricultural waste is pelletization. But hygroscopicity is one of the most important disadvantages of pellets. The initial pellets absorb moisture, swell and are destroyed at certain humidity. Also the heat value of biomass is less than the same parameter for traditional fossil fuels. Heat treatment in temperature range 230–280 °C in an oxygen-free environment

(torrefaction) allows to improve the characteristics of the solid fuel from agricultural waste. In this paper, the effect of heat treatment on the characteristics of the fuel from flax waste is presented. Torrefaction was carried out at three temperature values: 230, 250 and 270 °C. TG analysis, elemental (CHNS) analysis and measurement of hygroscopicity limit for initial and torrefied product were performed in the course of research. Heat value was calculated on the basis of elemental analysis results. With increasing of torrefaction temperature the limit hygroscopicity diminishes. Hygroscopicity limit was decreased almost three times for pellets, which have been torrefied at a temperature of 270 °C. Heat value was increased by 10% compared with the initial pellet on dry state. It is shown that the heat treatment leads to improved characteristics of flax pellets, namely an increase of the heat value and the hydrophobic properties.

Investigation of pyrolysis and torrefaction tar decomposition by thermal cracking

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Today the biomass processing as pyrolysis and gasification are actively progressed in developed countries. According to experts of the International Energy Agency the pyrolysis is the most universal, efficient, and cheap technology of the biomass energy use. The pyrolysis products of hydrocarbon raw material are carbon residue, non-condensable gases (CO_2, CO, H_2, N_2, and C_nH_m) and the pyrolysis liquid, which under normal conditions is a mixture of different acids, tars and water. Disposal of the liquid fraction is quite a serious problem for environment. The carbon residue is 20–40% by weight of the raw material, depending on the temperature of feedstock heating. Recycling of the liquid fraction leads to an increase of conversion degree of raw material to gas. In this paper

the processing method of the liquid fraction obtained by the high temperature and the low temperature (torrefaction) pyrolysis with use of thermal cracking is studied. The sewage sludge and chicken litter are used as raw material for experiments. Comparison of gas-mixture properties (volume, composition and calorific value) that can be obtained in various environments of the thermal cracking (charcoal, ceramic) is carried out. The deposition process of sulfur exiting from raw materials on charcoal heated to a temperature of 1000 °C is investigated. From results of experiments it is seen that the thermal cracking of the liquid fractions obtained by pyrolysis of biomass leads to complete processing of acid, tar, and water to mixture of non-condensable pyrolysis gas consisting of CO and H_2.
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Hydrothermal carbonization of vegetable biomass

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The interest in treatment of vegetable biomass is increasing in recent years. Vegetable biomass can be considered as renewable raw materials for realization a series of chemical and power processes grows. The resulting product—biochar has an increased energy density in contrast with biomass and can be exposed long-term storage and transportation. One of the modern methods of obtaining biochar from biomass is called hydrothermal carbonization (HTC). The process of biochar formation by HTC proceeds at temperature 220 °C and pressure 25 bar in the presence of water, without air and with the addition of catalyst. The distribution of products resulting from the HTC strongly depends on the type of raw materials and the reaction conditions. The benefits of HTC process is almost 100% "carbon efficiency", conditioned by chemical reactions occurring during the process, a high level of ecological compatibility of the

process and the possibility of processing wet biomass without pre-drying. The obtained carbon can be dewatered mechanically due to the hydrophobic properties. In this way, the final drying of biochar requires less heat in comparison with a classical pre-drying process, we can speak about a more economical method of biomass processing. At the Joint Institute for High Temperatures RAS, researching of process of the hydrothermal carbonization of biomass, on the basis of peat deposits Mayak of the Novgorod region, is started. Hydrothermal carbonization of peat led to decrease the release of volatile substances by almost 30%, increase the calorific value of 1.5 times and significantly reduce the moisture and ash content. Coal obtained during the experiment is close in its characteristics to fossil brown coal and the calorific value of coal is similar to black coal.

Estimation of solar energy resources for low salinity water desalination in several regions of Russia

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Access to fresh water becomes more and more crucial in modern world both for domestic and agricultural needs. For some southern agricultural-oriented regions of Russia the problem of poor water and energy infrastructure exists. Therefore, many of these regions possess local lowsalinity ground water and huge amount of sunny days. Reverse-osmosis desalination is suitable technology for local water desalination especially at low salinities. Usually under poor energy infrastructure conditions this technology is coupled with solar or wind energy in a case of sufficient renewable energy potential. Using regional data on ground water salinity from different sources and empirical dependence of specific energy consumption on salinity and temperature based on experimental results [1], estimations

for demanded photovoltaic (PV) array area and capital expenses to feed reverse osmosis desalination unit (1 m^3/h fresh water production rate) have been made for different regions of Russia. The most optimal results were obtained for Kalmyk Republic, Crimea Republic and Astrakhan region. Combination of salinity, temperature and solar radiation level there makes reverse osmosis coupled with photovoltaics very attractive technology to solve infrastructure problems in rural areas. Estimation results are represented as maps showing PV array area and capital expense level for the selected regions.

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Numerical modeling of torrefaction reactor with heating gas recirculation

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One of the principal ecological problems in the implementation of torrefaction technology in reactor with direct heating of biomass feedstock by flue gas is efficient utilization of vapor–gas mixture of heating flue gases and volatile torrefaction products. The problem is complicated by the low concentration of volatile products and a substantial amount of water vapor in the exhaust gas, which requires high energy expenditure for their utilization. The paper presents results of numerical analysis of energy-technological complex (ETC) including gas piston cogeneration power plant (GPU), torrefaction reactor with recirculation of heating gas and heat recovery boiler (HRB). The mathematical model of the torrefaction reactor [1] was supplemented by the conservation equation for the flow of volatile products and by the module, describing the recirculation loop of heat-transfer gas. On the basis of data on the composition of torrefaction volatile products [2] the temperature dependences of heat capacities for them and their combustion products as well as the

corresponding combustion heat values were calculated. Calculations of the reactor without recirculation and with recirculation of the heating gas in torrefaction zone at a different frequency of torrefied biomass discharge were held. It is shown that in recirculation modes the concentration of volatile products at the reactor outlet is increased by almost an order. Also GPU power, required for providing given reactor productivity, is reduced several times and the consumption of natural gas, needed for post-combustion of volatile products in HRB, is reduced by an order, significantly increasing the energy efficiency of all ETC.

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Modeling power loads using a neural network

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While solving the problem of optimizing operation modes and the composition of the equipment of small power complexes and a number of other tasks related to energy planning, it is necessary to have data on the graphs of the consumer's loads. The characteristic calculation horizon is 1 year with hourly sequences of load changes. Usually, there is a lack of reliable information about energy consumption dynamics and simulation should be used. In recent years, many Russian and foreign journals published a number of works devoted to various approaches to the modeling of energy loads. Such works usually suggest splitting consumers into groups with specific allocation of load graphs and analysis with further mathematical model creation. Many various mathematical apparatuses are offered for the analysis: Fourier series, statistical methods, artificial neural networks, etc. The latter method is the most interesting and promising due to the flexibility, low insistence to the number of input data and the possibility of virtually infinite perfection of the network by

extending the training sample. The paper discusses the features of several key energy consumer groups, which often have autonomous power supply: residential buildings, agricultural enterprises, light industries and food industries. The structure of the neural network for simulating the load charts of different consumers is suggested. The simulation results using a neural network and using the Fourier series expansion are present.

2. Shock Waves, Detonation and Combustion

New data on the kinetics and governing factors of the spall fracture of metals

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In studies of the spall strength of metals, its dependences on the strain rate and in some cases on the peak shock pressure are usually determined. As a result of constrained fracture rate the spall strength value grows with increasing the rate of loading. Concerning the peak stress in preceding shock wave, it was reported about both independence of the spall strength of the peak stress and about growth of the spall strength with increasing the peak shock stress. In our talk we shall present two examples of significant departures from these trends. In experiments with vanadium single crystals we observed essential decrease of the spall strength with increasing the shock stress that was interpreted in terms of disruption of the matter homogeneity as a result of its twinning at shock compression. In the experiments with 12Kh18N10T austenitic stainless steel we observed sharp increase of recorded spall strength value when short load pulses of a triangular profile were replaced by shock pulses of long duration having trapezoidal shape. This anomaly is associated with formation of the deformation-induced martensitic phase which increases the yield stress in the vicinity of growing pores. Depending on the strain rate, the effect emerges in different stages of the spall fracture. This study was supported by the State Corporation "Rosatom" (state contract N.4kh.44.9B.16.1012, March 01, 2016).

The simple wave metamorphosis in the channel

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The simple (Riemann) wave is supposed to retain its properties while running in a channel, for example, by driving of gas before the piston. However, the pipe walls (and of a channel in general) significantly change the nature of the flow. The loss of kinetic energy of moving gas due to viscous friction on the wall compensates the piston which generates impulses. These impulses form a sequence of compression waves within the flow. Since the velocity is zero on the walls, the local pressure rises by virtue of the of the energy conservation law. A zone of the local high pressure propagates into the stream as a perturbation in the form of an acoustic wave of spherical shape, which carries the fluctuation of gas velocity [1]. A set of the waves and their reflections from the walls creates the field of spatiotemporal oscillations within the flow. Energy of the oscillations is small, only a few percent, however, when the flow velocity grows, these become noticeable and are referred to as the turbulent. Also, the flow in a channel of restricted cross-section size should be considered as the wave beam susceptible to diffraction divergence [2] that transforms a flat wave front in spherical segment. Wave type the spherical segment and their reflections from the walls form a mode structure of oscillations, as in a conventional waveguide. In other words, dissipation caused by viscous friction and wave beam divergence violates condition of self-similar flow, and the term "Riemann wave" in the channel can be applied only very conditionally. At the same time, the change for the simple wave propagation conditions give opportunity to release and explain cause for such phenomenon as the turbulence, for example [3].

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Stability of shock wave structures and uniqueness of solution to the Riemann problem for the generalized Hopf equation

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The Korteweg–de-Vries–Burgers (KdVB) equation is proposed as a prototype of partial differential equations with dynamic discontinuities (shock waves). Depending on the relation between the parameters of dispersion and dissipation, the KdVB equation with a special non-convex potential can have a finite number of types of stationary solutions representing structures of special discontinuities (i.e. discontinuities with extra relations following from the demand for structure existence). The number of such special discontinuities of different types grows as the relative influence of dispersion is enhanced as compared with dissipation. This causes multiple non-uniqueness of solutions when these discontinuities are used to construct solutions of self-similar problems [1].

We give detailed analysis of the steady travelling wave solutions from a viewpoint of discontinuities. An Evans function formulation to study the linear stability is used. Integrations of the initial value problem illustrating the instabilities are presented. Relying on the results of [2, 3] we construct a self-similar solution of the problem of arbitrary discontinuity disintegration. This solution consists of only discontinuities with a stable stationary or non-stationary structure. A final criterion is formulated for choosing an admissible discontinuity (discontinuities) to be the result of the Cauchy data evolution in the problem of arbitrary discontinuity disintegration.

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Method development for measuring dynamic strength properties of concretes under shock pulses with duration from a few to tens of microseconds

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Several schemes for the organization of measurements the dynamic strength of concrete using explosive devices with generation of long duration compression pulses in planar samples (uniaxial deformation) and the rods (uniaxial stress state) have been tested. The main results are obtained in experiments with concrete rods of diameter from 28 to 100 mm. Under uniaxial shock compression, the elastic-plastic wave with a weak jump on the front of the elastic precursor and a long rise time at plastic wave is formed. Spall strength of the concrete is less than 20 MPa. Under explosive loading the concrete, sample failure occurs on the initial section of the wave propagation, when a rapid drop in the peak compressive stresses is observed. The rest of the rod remained in the intact form of several parts separated by a surface of the spall. In this area a blur and slow decay of a pulse of elastic compression occurs. Measurements of compressive stress at the border of the failure zone allow to determine the value of the dynamic strength of the concrete, which turned out to be four times higher than the static strength and slightly varies with the change of the diameter of the rod. This work was supported by the State Corporation "Rosatom" (N.4h.44.9B.16.1012, March,1, 2016).

Using of W–Cu-alloys for shock synthesis experiments: A pathway to the 2 Mbar boundary?

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To reach the 2 Mbar boundary with shock synthesis experiments under the requirement of complete sample recovery and to obtain recoverable high pressure phases in this pressure range it will be required to reduce the shock temperature simultaneously with every step which will increase the pressure. This is strictly required to avoid any overheating of the sample (the so called "Knudson-problem" [1]), defined by the separation of the Hugoniot from its isentrope. For this reason the Shock Wave Laboratory Freiberg works only with the reverbration method in the pressure range beyond 1 Mbar. To reach 2 Mbar and to obtain phase transformations under earth core conditions additionally temperature reducing will be required and this problem is not solved yet [2]. For this reason a method was developed to obtain up to three indepenedent reverbration horizons in the recovery capsule based on heavy W–Cu-alloys. An overview about the behavior of this for shock experiments new mechanical alloys will be given.

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Flyer acceleration by magnetic pressure on Angara-5-1 installation

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The high pressure created by magnetic field which was induced by the current flowing through the flyer allows one to reach the megabar pressures and to accelerate the flyers to high velocities. For intense impact of this flyer onto the studied substance it is necessary that a significant portion of the flyer had the density close to the density of the solid. But a part of the stored energy would be spent to the Joule heating and the formation of the shock waves in the flyer. The effectiveness of the flyer acceleration was studied on the Angara-5-1 installation at the linear current density up to 5 MA/cm.

The experimental and numerical study of the evolution of the aluminum flyer under flowing of the sub-microsecond megaampere current pulse with the linear current density up to 5 MA/cm through it was carried out. It was obtained that by the time 500 ns the substance of the flyer near its back surface and at a depth of about 300 μm is in the solid state, and the velocity of the back surface by this time is 10 km/s.

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The measurement of liner brightness temperature by optical spectral method

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The brightness temperature is one of the parameters characterizing the state of the liner cylindrical surface when strong shock wave output on a metal free surface [1–4]. Its measurement in a large-scale experiment presents certain difficulties. This paper presents a method for measuring of brightness temperature of axially compressible liner by optical spectral method. For temperature recording used an optical spectral channel, it made and tested in IPCP RAS. To obtain absolute values of the radiation intensity was calibrated the measurement channel of optical system using xenon and tungsten sources. The paper presents three ways of measuring the brightness temperature of the surface for large-scale explosive experiments at wavelengths of 620 and 850 nm. By means of presentation techniques were estimated brightness temperature and the average speed for copper and steel liners compression by detonation products. This work was supported by the Program of the Presidium of the Russian Academy of Sciences "Thermal physics of high energy density". The work was carried out on the equipment of Interregional Explosive Center for Collective Use.

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Electrical conductivity and equation of state of vitreous selenium under shock compression

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Experiments on measurement of vitreous selenium conductivity in the conditions of step-like shock compression up to 45 GPa are executed. Samples for researches represented a tablet with a diameter of 10 mm and thickness 0.5 mm, pressed to density of 3.9–4.1 g/cm^3. In one plane with a sample the manganin pressure gauge settled down. Pressure in experimental setup was generated by the aluminum plate accelerated to the speed of 2 km/s. The design of a measuring cell was similar to [1]. The semi-empirical equation of state of vitreous selenium has been developed for calculation of thermodynamic parameters of a sample. With use of the equation of state numerical modeling of experiments is carried out, data on thermodynamic history of sample loading are obtained. It is shown that sample conductivity increases on several orders of size and grows synchronously with a step-like profile of pressure in experimental setup.

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Superconductivity in Al–Al_2O_3 interface

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It is known that in granular Al thin films the superconducting transition temperature, T_c, can be nearly twice as much as $T_c \approx 65$ K of bulk Al. It was discovered that the films with comparable grain size, evaporated either at low temperatures in oxygen-free ambience or at room temperature in oxygen atmosphere, demonstrate similar enhancement of the T_c (compared to that in the bulk). This fact suggested a conclusion that aluminum oxide itself does not participate in the T_c-enhancement mechanism. Moreover, the films evaporated at low temperatures restore the bulk value $T_c \approx 1.2$ K after room-temperature annealing, while those evaporated in oxygen survive room-temperature storage with unchanged T_c. Thus, the only role of oxygen has been considered to stabilize the fine-grain structure of the film, conserving small aluminum grains with aluminum oxide coating, which results in stabilization of the enhanced T_c irrespective of exposure of the film to the normal conditions. Metastable superconductivity at $T_c \approx 65$ K has been observed in Al foil subjected to special oxidation process, according to the ac magnetic susceptibility and electrical resistance measurements. Comparison of the ac susceptibility and the dc magnetization measurements infers that the superconductivity arises within the interfacial granular layer formed during the oxidation process between metallic aluminum and its oxide.

Experimental study of shock wave compressibility of fiberglass

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Using a laser interferometer VISAR with a nanosecond time resolution the experiments on investigation of shock compressibility of heterogeneous anisotropic material fiberglass were conducted. Fiberglass is a polymeric composite material consisting of interwoven fibers from glass and an epoxy matrix. A feature of this material is a strongly pronounced anisotropy of properties. The shock wave profile and the shock wave velocity of fiberglass were obtained in each experiment. Two-wave configuration almost in the entire pressure range was recorded for both orientations of the fibers. But amplitude of precursor along the fibers (about 100 m/s) is much higher than the amplitude for the transverse direction. From the obtained experimental data Hugoniots of fiberglass for two orientations of fibers were plotted in the coordinates of the shock wave velocity D–particle velocity u. Within the error Hugoniots for both directions coincide ($D = 1.85 + 1.1u$ km/s). Also a study of spall strength for fiberglass was conducted. It was shown that the value of spall strength for parallel orientation of the fibers is in the order of magnitude higher than for perpendicular orientation, which is equal to 12 MPa. From the obtained in this work results it can be concluded that the correct description of the dynamic deformation of anisotropic material fiberglass is possible only within the framework of the two-component model considering the real motion of the fibers and their interaction with the matrix.

The work is carried out with the financial support of FAIR–Russia Research Center.

Pulse compression and tension of porous materials under shock-wave loading

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The paper presents new experimental data on the properties of porous media under shock-wave loading and on the spall strenght of the samples made on the basis of the rubber matrix. The porosity of the samples was created with the filler made of glass microspheres. The first set of the samples featured the particles about 80 μm in size; the second set of the samples featured the particles sized within the range from 20 to 150 μm. The velocity profiles of the samples, subjected to shock-wave loading, were measured with VISAR laser Doppler interferometer. The obtained profiles have rather complex structure of the shock-wave front; such structure is created by the pores collapse kinetics in the investigated heterogeneous samples. The profiles show a two-wave configuration which is most distinctly seen at low pressures. As a result of processing of the experimental data there were obtained the Hugoniots for the materials at high pressures and some data on the substance isentrope at low pressures. The two-wave configuration areas turned out to be different for the investigated materials, this difference being caused by the dependence of microspheres collapse threshold on the microspheres concentration and size. The experiments show that the rubber with microspheres is a material featuring low damage threshold under pulse tension. The work is carried out with the financial support of FAIR–Russia Research Center.

Dynamic response of molybdenum to ultrafast laser induced shocks

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Molybdenum is a bcc transitional metal whose high-pressure behavior has attracted considerable experimental and theoretical interest. In the present paper chirped pulse interferometry was applied to study ultrafast shock waves evolution with 1 ps temporal resolution in molybdenum submicron film samples under loading up to 40 GPa created by a femtosecond laser. The new data on Hugoniot elastic limit on a submicron propagation distance and shear stress was obtained. Also the spall strength of molybdenum in a condense state at the strain rate of 10^8 c^{-1} was estimated and morphology of damage was investigated using scanning electron microscopy.

Amorphous carbon and rhombohedral graphite during fracture of diamond under contact with liquid carbon

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Diamond in polishing and indentation processes as well as being compressed in diamond anvils without soft gasket destroyed plastically due to conversion of diamond to other forms of carbon. Previously, graphite and amorphous carbon (a-C) was found in destroyed

diamonds, but the reasons for the formation of one or the other carbon phases had not been established.
We made a brief contact of diamond with liquid carbon and compare the structures of carbon in various areas along the length of one of the crack among themselves and with the structures of the faces that surround the crack by using high-resolution transmission electron microscope. We conclude that (i) crack is fully filled with rhombohedral graphite and a-C which are not mixed, (ii) the a-C adjacent only to the partially graphitized diamond of the crack face, (iii) faces of the crack are deployed relative to each other.
Thus the non-diamond carbon is formed as a result of the elastic energy relaxation stored in the region of the crack. Hard face of the crack gives smaller relaxation rate and crystalline carbon, while softer partially graphitized face crack will provide fast relaxation and less ordered a-C.
The destruction on brittle mechanism must be considered in experimental determining the spall strength of diamond. Also one can make a practical conclusion that the more delicate polishing of a diamond happens when you saturate the surface layer with graphitization catalysts, for example boron.

Multiscale investigation of dynamic fracture of metals and metal melts

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Tensile fracture takes place at a compression pulse reflection from a metal free surface that leads to arising of a tension wave with negative pressure leading to fracture. Similar phenomenon is observed in metal melts. With the help of the molecular dynamics, we develop a continuum model of the tensile fracture of solid metals with accounting of initial voids, inclusions [1], dislocations and grain boundaries. The model includes the kinetic equations for formation, growth [2] and interaction of voids. It is verified by means of comparison with

the taken from literature experimental free surface velocity histories for the high-velocity plate impact problem. In similar manner we develop a continuum model of the dynamic fracture of metal melts, both initially homogeneous [3] and with initial voids or inclusions [4]. The molecular dynamic investigation of the late stages of fracture of both solid and molten metal shows that material reaches the tensile strength much earlier the complete fracture. The work required for complete fracture in the form of fragmentation exceeds several times the work on reaching the maximal tensile strength [5]. The proposed models of fracture are used for numerical modeling in the problems of the high-velocity impact or the high-current electron irradiation of metals. The main part of this work was supported by the grant from the Russian Science Foundation (project No. 14-11-00538); investigations for magnesium was supported by the grant from the President of the Russian Federation (project No. MD-7481.2016.1).

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Different physical nature of strain rate sensitivity of metals and alloys at low and high strain rates

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Strain rate sensitivity parameter is traditionally used to describe the changes in the yield strength of materials at increasing the strain

rate. At the same time, at high strain rates, there are additional effects of the material strain softening associated with an increasing in the density of mobile dislocations and reducing the dynamic yield stress [1]. The nature of this effect remains a scantily explored issue. We consider the phenomenon of micro-localization at the shock front in aluminum by three independent positions: using dislocation plasticity based numerical simulation [1, 4], the integral criterion of plasticity [1, 3] and comparison with the experimental measurements of the particle velocity dispersion [4]. It allows us to relate the amount of deformation intensity deviation with the mechanical parameter of the strain rate sensitivity and, thus, determine the class of materials to which these instabilities are mechanically significant. The study was supported by grants from the President of the Russian Federation (MK-4649.2016.1 and MD-7481.2016.1) and the Russian Foundation for Basic Research (16-31-60051).

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Tensile strength of Fe–Ni and Mg–Al nanocomposites

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With the use of the molecular dynamics simulations, we consider two perspective materials for various applications. They can have better properties (stiffness, specific shear strength, etc.) in comparison with a pure material of matrix. In addition to interest for this investigation, these materials have different mechanism of fracture. The first mechanism is connected with a stress concentration in matrix (Mg) near a stiff and strong inclusion (Al); in this case, the fracture occurs inside the matrix and does not touch the inclusion. The second mechanism is connected with atoms disorder along

surface of inclusion (Ni); in this case, the less energy is required for the voids formation in the area near at the inclusion surface.
The strength of the considered systems weakly depends on the orientation of crystal lattice of inclusions relative to the tension direction. The tensile strength of Fe–Ni and Mg–Al systems is determined at varied strain rates (in the range from 0.1/ns to 10/ns at the temperature 300 K) and varied temperatures (in the range from 300 to 1100 K at the strain rate 1/ns). The rate sensitivity of strength of a material with inclusions is higher than that for a material without inclusions.
We propose a continuum model of the nanocomposite fracture that is based on the equations of nucleation and growth of voids; the model takes into account the stress concentration around inclusions. A comparison with the molecular dynamics results shows that the continuum model allows us to describe the rate and temperature dependences of the nanocomposite strength at least for strain rates 0.1/ns.

Mechanical and structural characterization of polyethylene-based nanocomposites with carbon reinforcements under tensile deformation

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Nowadays glassy polymers are the interesting subject in materials science due to their exceptional mechanical properties such as expansivity or viscoelastic. It is of the great interest to establish the behavior of glassy polymers on adding carbon nanotubes to their

molecular structure [1]. Molecular dynamics (MD) gives the opportunity to build this model with great predictable capabilities. In this work we discuss the results of MD simulation of glassy polymer with multiwall carbon nanotubes under tensile deformation. We use primitive path (PP) [2] analysis to study the evolution of entanglement structure of polymer chains under the tensile deformation. Besides the mechanical properties of the material attention is given to the accuracy of MD computation using the power of high-performance supercomputer.
The work is supported by the Russian Science Foundation (grant No. 14-50-00124).

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Study of high-rate cooper strain by split Hopkinson bars method

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Dynamic strain of materials is studied for more that half a century. However such investigations result in different, often hard-comparable characteristics. Reliability and comparability of investigation results is defined, first of all, by scientific validation of high-speed material test setup. One method having clear theoretical basis, high efficiency, universality and reliability of the obtained results is the split Hopkinson bars (SHB) method or Kolsky method. This method falls with in the class of tests with consonant strain

rate e=const; it allows one to study dynamic diagrams of compression and tension under strain rates e=10^2-10^4 s^{-1}. Method modification make it possible to study adiabatic shift, crack resistance, Bauschinger effect and other dynamic characteristics of materials. The paper describes the teat installation using SHB method and presents the results of experiments in cooper. Strain diagrams, obtained during the experiments, demonstrate high accuracy and repeatability of results. Based on the obtained results the parameters of cooper strain in Johnson-Cook from were defines. The derived constitutive equation in Johnson-Cook from may be expected to improve accuracy of describing cooper dynamic strain in numerical simulation of shock-wave processes.

Effects of elastic-plastic behavior of materials on the nature of wave formation during explosion welding: Numerical simulation

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Explosive welding is an effective method of joining of various metals and alloys with very different strength and thermophysical properties. In this work we continue the numerical simulation of explosion welding process in elastic-plastic approximation [1], under study were the peculiarities of bonding formation by the explosive welding of metals with highly differing properties (steel–carbide composite and copper–hardened steel). In experiments [2] one can see the waves typical for the explosion welding on the copper–steel interface, whereas the interface of the stainless steel and carbide composite is flat, there are no waves, which is natural for the welding of the materials with highly differing strength parameters. The results of numerical simulation of wave formation during explosion welding are presented.

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Shock-wave-induced plastic deformation of surface nanorelief or deposited nanoparticles

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Reflection of a shock wave from a free surface generates a tensile wave, which can induce a spall fracture. In the case the free surface has a nanorelief in the form of deposited nanoparticles, protrusions or cavities comparable in size with the shock wave thickness the compression pulse action causes a severe plastic deformation of the surface nanorelief elements. On the one hand, a part of the compression pulse energy is dissipated that reduces the tensile wave and increases the spalling threshold [1, 2]. On the other hand, a compaction of the surface layer occurs. The first effect can be used to increase the spallation resistance, and the second effect can be used to secure the deposited nanoparticles in the form of a film. We present the molecular dynamic simulation results for the interaction of picosecond compression pulses with a flat surface and a surface with deposited nanoparticles or protrusions. The compression pulse is excited by either a flat impactor or consequent applying of pressure pulses to the front surface of the investigated sample. We investigate for aluminum and copper samples the dependence of the minimal shock wave amplitude resulting in spallation from the nanorelief characteristics. Also we determine the conditions for a nanoparticle layer compaction into a monolithic coating by means of plastic deformation initiated by the compression pulse.

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Simulation of cylindrical and spherical shell collapse with considering dislocation plasticity of metals

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Experiments on collapse of cylindrical [1] and spherical metal shells are used for researching the deformation behavior of metals in the conditions of energy cumulation in the converging shock wave. A significant experimental material has been accumulated currently, including the data of metallographic researches [1]. The modeling of this process is usually carried out in the hydrodynamic approximation or with using the simplest models of the elastic-plastic behavior of metals. More realistic models include a description of the evolution of structural defects in the material, for example dislocations. In this work, we perform modeling of the collapse of the cylindrical and spherical aluminum shells. Continuum mechanics equations are solved numerically in the one-dimensional cylindrical and spherical formulations with using the numerical method [2]; the substance behavior is described by using the of dislocation plasticity model [3,4]. This work is supported by the Ministry of Education and Science of the Russian Federation (project 3.2510.2017/PP).

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Two scale modeling of high rate plasticity of aluminum containing nanometer sized θ' phase

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In this work the atomistic simulations of dislocation overcoming of nanometer sized θ' phase for different temperature are performed. The law of dislocation motion in the crystal with hardening centers is formulated through the fitting with the molecular dynamics results. The obtained law is further incorporated into the continuum model of dislocation plasticity. The continuum calculations of shock wave propagation in aluminum with θ' phase are carried out in comparison with the previously modeled pure aluminum and aluminum containing Guinier–Preston zones and, also, with the experimental results.

Analysis of parallel molecular dynamics for MPI, CUDA and CUDA-MPI implementation

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One of the most difficult issues in molecular dynamic modelling is a large computation time of the task even for relatively small systems of atoms. The main method of solving this problem is implementation of highly efficient parallel codes. In the framework of current

study three implementations of parallel MD algorithms were compared. The first approach was based on design of highly parallel program for a computer cluster with distributed memory using Message Passing Interface (MPI). The second type of parallel algorithms was implemented on CUDA based General Purpose GPUs by NVIDIA. It should be noted, that modern high performance computing systems are a combination of MPI clusters equipped with GPGPUs, what turns them into so-called heterogeneous computing clusters. In this case MPI technology is used for internode communications, while all computations are carried out by GPUs. Thus, the third approach to the parallelization discussed in this study was based on design of a CUDA-MPI algorithm. The detailed studies and comparison of all three approaches (MPI, CUDA and CUDA-MPI) were performed in order to define optimal parameters and conditions of applicability of each algorithm.

Dislocation mobility calculation in bcc molybdenum using method of molecular dynamics

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Nowadays plastic properties of metals are considered to be governed by dislocation movement. Hence dislocation behaviour and dislocation structure have been the subject of plenty experimental and theoretical research [**?**, 1, 2]. However, it is challenging to study behaviour of a single dislocation in experimental research because one have to reach high resolution and manage to introduce a single dislocation in crystal [3]. Therefore it is more convenient to study single dislocation behaviour using method of molecular dynamics which has already shown good results in simulation of atomic-level processes. In this work we perform molecular dynamics simulations

of dislocation movement under applied shear stress in molybdenum in order to estimate mobility of dislocations.
In this work we created atomistic models of screw and edge dislocations in molybednum with periodic boundary conditions through 2 dimensions. Using these models, we performed mobility calculations by estimation of velocity dependency on applied shear stress. The results show that screw dislocation is less mobile than edge which is in a good agreement with experimental data. In addition results was approximated by mobility functions which are input data for dislocation dynamics calculation.

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Smooth-particle hydrodynamics simulated boron carbide failure under shock compression

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Boron carbide response to shock compression, large strains, and high strain rate is of the present-day interest. Due to unique strength properties of material it has numerous applications. Nevertheless, under shock loading boron carbide is involved into a proccess of failure [1] what significantly reduces its strength as demonstrated in plate-impact experiments [2].
Boron carbide failure process under shock compression is investigated by comparison of smooth-particle hydrodynamics [3] simulations with two sets of plate-impact experiments where samples manufactured using different technology [2, 4]. Different boron carbide

failure models are applied to determine relevant physical properties which influence wave profiles obtained by VISAR measurements. The strength at the failed state of material is demonstrated to be different in considered experiments independently of particular model.

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The tool for high-velocity interaction and damage of solids

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The basic steps for creating a numerical tool to simulate the deformation and failure processes of complex technical objects (CTO) are presented. Calculations of shock loading of CTO both at low and high speeds, showing the efficiency of the numerical tools created are carried out.

Simulation of deformation and failure of complex technical objects at impact requires a numerical tool allowing one to examine possible scenarios of their development in real time.

Reactor2D allows for solving nonstationary tasks of deformation and failure of CTO and includes the following steps: Mathematical formulation of equations of mass balance, momentum, and energy; Setting the initial data and formulation of the boundary conditions for all CTO elements; Choosing the equations of state and the equations of process for all the CTO materials [1, 2]; Determining the necessary criteria for destruction of the materials, covering a variety of mechanisms of their destruction [3]; Constructing geometric images of all the CTO elements and filling their difference grids [4]; Constructing a symmetrical algorithm for calculating the contact

boundaries [3]; Modeling of fragments of the destroyed material by discrete finite-size particles.
The work is financially supported by the Russian Science Foundation, grant No. 16-19-10300.

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Comparative study of shock pulse evolution in aluminum and polymethylmethacrylate

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Powerful short-pulse laser irradiation generates compression pulse, which consists of a shock wave and a following release wave. Propagation of this pulse through material imposes plastic deformation and microstructure change, while its reflection in the form of tension pulse can lead to spall fracture. Both the microstructure change and the fracture are sensitive to the shock amplitude. It had been shown in [1] on the basis of dislocation plasticity model that elastoplastic properties significantly influence the shock wave evolution. The compression pulse had been generated by high-velocity plate impact. On the other hand, it had been shown in [2] on the basis of Maxwell model that there is no significant effect of viscoelastic properties on the compression pulse attenuation in polymethylmethacrylate (PMMA). The compression pulse had been generated by a pressure pulse applied to sample surface. Purpose of present work consists in a more detailed investigation of the viscoelastic properties influence on the compression pulse evolution in metals by an example

of aluminum and in polymers by an example of PMMA. The results not only allow one to separate the influence of material from the influence of the pulse parameters, but also reveal the parameter range, within which the viscoelastic properties should be taken into account for correctness of calculations of the compression pulse dynamics.

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Mathematical modeling of two metal plates impact using two-phase approach

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The goal of the work is the numerical investigation of two metal plates impact in the statement from [2] using two-phase compressible model [2]. In one-dimensional case the governing system of equations comprises seven equations: three conservation laws for each phase and transfer equation for the volume fraction of one of the phases. Both phases are considered to be compressible and non-equilibrium on velocities and pressures. The system has hyperbolic type but couldn't be written in the conservative form because of nozzling right-hand side terms. The computational algorithm is based on the Harten-Lax-van Leer numerical flux function. The robust computation in the presence of the interface boundary is carried out due to the special pressure relaxation procedure. The problem is solved using stiffened gas equations of state for each phase with the parameters calibrated using the data obtained with the use of wide-range equations of states for the metals. In simulations we

got two shocks after the initial impact which propagate to the free surfaces of the samples with the parameters within the range of percents of error in comparison with wide-range equations of states computations.

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Numerical simulation of the shock waves propagation in elastic deformable tube with variable wall thickness

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The shock wave propagation in a long elastic deformable pipeline is accompanied by a number of strongly multidimensional effects. First of all, it concerns the "breathing" of the pipe (diameter change) at its loading by pressure waves. This factor can strongly influence quantitative and qualitative characteristics of flow. In this paper we consider the isothermal flow of weakly compressible liquid. The movement is considered in the tube with the elastic deformable wall, which allows the flow to expand with a pressure increase. To describe the behavior of such a system a system of equations for the one-dimensional unsteady flow was used. To describe the behavior of the tube wall we used the following assumption: at each instant each annular elastic tube element is in equilibrium with the pressure in the corresponding cross-section. According to the above approach it has solved the problem of shock wave propagation in tube with variable wall thickness. The wall thickness varied sinusoidally with a very long period. The shock wave generated by an instantaneous water hammer. As a result, shock wave propagates in the tube with essentially oscillating pressure profile. It is interesting to note (and we can not explain this fact), that the period of oscillation

of the liquid column behind the shock wave does not coincide with the period of the wall thickness variation, The calculations show that the spatial size of the periodically oscillating liquid column is twice the period of the change in the thickness of the pipe walls. This work was supported by the Russian Science Foundation (grant No. 16-19-00188).

Peculiarities of structural transformations in metal nanoparticles at high speed collisions

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A molecular dynamics simulation of nanosized particle collision under the electrical explosion of metal wires of different types was conducted. Interatomic interactions were described on the base of the embedded atom method. Used potentials allowed describing with high accuracy many mechanical and physical properties which are very important for the simulations of nanoparticle collisions with high velocities. The dynamics of the nanosized particle formation synthesized at the non-synchronous electric explosion of metal wires of different types was studied. Features of particle collisions on the example of nanoscale particles of copper and nickel, whose speed varied from 50 to 500 m/sec were investigated. The temperature of the particles synthesized by the collisions was decreased to room temperature by scaling of the atomic velocities. The peculiarities of structural transformations in the colliding particles depending on the speed of collision were determined. The intervals of collision velocities in which interaction between particles is elastic or leads to the formation of structural defects or melting were calculated. The analysis of the structure and distribution of chemical composition over the cross section of the particles which were synthesized under simultaneous explosions of different metal wires was carried out.

The work was performed with financial support of Russian Foundation for Basic Research grant No. 15-01-06585.

Structural and morphological transformations of amorphous glassy carbon under high shock pressures

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The basic part of carbon atoms in amorphous glassy carbon (GC) is in the sp^2–hybridizations. Recently interest has raised to behaviour of GC at high pressures and temperatures in connection with its possible transformations into superhard carbon materials. So GC transforms into new superhard material—amorphous diamond in diamond anvils under pressure 44 GPa [1]. This process has appeared reversible, that is after pressure amorphous diamond came back in glassy carbon. At the same time under static compression at high temperatures the stable form nanocrystalline diamond can be received [2]. At last, in [3] glassy carbon has been used for synthesis of lonsdaleite in the warmed diamond anvils and the high shift deformations.In the given work the morphological and structural transformations of glassy carbon were studied at high multiple shocks.The experiments have been carried out with recovering of GC samples after strong multiple shock in the 0–100 GPa pressure range. The spectroscopic and morphological (optical and electronic microscopy) analysis is executed for products of structural transformations which were stimulated by high shock pressures. Reconstruction of thermodynamic history of samples of glassy carbon out of recovering ampoules is carried out also. The thermodynamic history is correlated with transformations of shocked glassy carbon. This work is supported by the Russian Foundation for Basic Research (project No. 16-08-00237).

[1] Lin Y et al, 2011 *Phys. Rev. Lett.* **107** 175504

[2] Solopova N et al, 2015 *J. Cryst. Growth* **412** 54–59
[3] Shiell T B et al, 2016 *Sci. Rep.* 6:37232

Conductivity and equations of state of shocked beta-rhombohedral boron in megabar pressure range

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The finding of pressure dependence of specific electroconductivity for shocked boron was the purpose of work. Electroconductivity of shocked boron samples is measured in the area of multiple shocks pressure up to 100 GPa where various high pressure phases of this element exists. The equations of state of beta-rhombohedral and amorphous boron are constructed in a megabar shock pressure range.

Thermodynamic states of boron are calculated in the executed experiments. Calculations and the results of measurements have allowed to find the change of specific conductivity of boron at strong multiple shocks compression in the dynamic pressure up to 110 GPa and temperature up to 800 K.

It is shown, that at strong multiple shock compression the specific conductivity of boron increases from 10^{-5} $(\mathrm{Ohm\,cm})^{-1}$ up to 10^{+3} $(\mathrm{Ohm\,cm})^{-1}$.

The increase in the electrical conductivity of polycrystalline boron in the 100 GPa interpreted as a consequence of transition non-metal-to-metal.

It is shown that the pattern of change of the conductivity of beta-rhombohedral boron in the multiple shocks cycle compression and unloading has hysteresis.

This study was supported by the State Corporation Rosatom (contract No. N.4kh.44.9B.16.1012, March 01, 2016).

Experimental investigation of microwave radiation generated by explosion

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Generation of microwave radiation at a detonation of condensed explosives was repeatedly observed in many laboratories of the world. In 1998 a mechanism of such generation has been offered [1]. According to this model the layer of ionized gas behind an air shock wave forms a resonator, and products of detonation form a strongly nonequilibrium active medium, the oscillatory temperature in which essentially exceeds rotational temperature. In process of expansion of detonation products the concentration of electrons behind a shock wave will decrease, and microwave radiation will fall outside the limiting resonator. According to this model radiation should be registered with a certain delay with regard to the moment of the output of detonation wave on surface of charge. The conducted experiments confirm this conclusion of the theory. Measured delay-times are in agreement with theoretical estimations.

[1] Cherepen A and Shumilin V 1998 *Journal of Radio Electronics* **1**

Modeling results for two-staged magnetic cumulative generator with the fast open switch

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To generate an electrical pulse with the sharp front increase, two-staged magnetic cumulative generator (MCG) can be used. In addition, the open switch is useful and can be applied in a new power supply device, due to the fast increase of the output current in the beginning of MCG end stage run. The MCG numerical modeling is presented, with a primary circuit being switched off. The computer simulation has shown good output parameters of MCG under consideration. The power supply efficient of small-sized MCG will require additional experiments.

Pulse magnetic welding

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The quest for asserting pulse-power as the new industrial technology continues in this paper, describing the theory, test, and practice made towards creating viable processes where conventional means or production methods are replaced by pulse-power systems, with improved commercial results. Methods and means described in previous works come together to form practical system for sustained

production. Pulse magnetic welding is rated among the best methods for welding tubular parts, and is especially suited for aluminum alloys and for pairs of different metals, but it is also a most intricate one. This paper presents research results of implosive acceleration of tubular details using pulsed magnetic field, and numeric data of real industrial application. Two types of modular pulse current generator designs ware developed as well as methods to optimize working coil design. Calculated and measured distribution of magnetic field in various coils and field-shapers was reported in earlier work, and also the influence of coil material on technological results. The work-coils discussed work at industrial regimes, use water-cooling, and reach 50 000 pulses without fail. A method for measuring part speed during deformation was developed, and the speed of part investigated at real processes. The experimental results show good agreement with models, forming a base for industrial process design.

Interaction of debris with elements of spacecraft

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In this study, we carried out theoretical and experimental study of the interaction of high-speed compact and elongated strikers with barriers of finite thickness of the glass and asbotekstolit. These materials are used as elements of the spacecraft structure: windows, optical instruments, glasses, heat shields, etc. We consider the collision with aluminum particles simulating space debris and particles of ice and granite, modeling natural particles of cosmic bodies.To calculate the elastic-plastic flows used technique implemented on the tetrahedral cells and based on shared Wilkins method for the calculation of internal points of the body and Johnson method for calculating contact interactions. The process of breaking glass, ice, granite was considered as the process of breaking a brittle material, no portion of plastic deformation characteristic of the deformation

of metals. When solving problems in three-dimensional statement takes into account the heterogeneity of the natural structure of real materials, which affects the distribution of physical and mechanical characteristics in terms of structural elements and which is one of the factors determining the nature of the destruction of the latter. The account of this factor in the equations of mechanics of solids is possible in the application of the laws of probability distribution of physical and mechanical characteristics in terms of the structure under consideration. The initial inhomogeneity of the material takes into account the probability distribution of the criterion of destruction of the cells of the computational domain with a modified random number generator, issuing a random variable subject to the chosen distribution law.

Numerical modelling interaction of shells and the aircraft engine with concrete protective designs

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The numerical research destruction of concrete designs at interaction with various types of shells and an aircraft engine is conducted. Modeling is carried out on the basis of the author's computing code EFES. As concrete designs protective covers of nuclear power plants and concrete overlappings of underground constructions are considered. In calculations real schemes of reinforcing, availability of explosives in shells are considered. Schemes of development of destruction in concrete designs depending on geometrical and kinematic conditions of interaction are investigated.

The work has been conducted with the financial support of Russian Foundation for Basic Research (project No. 16-31-00125; project No. 16-38-00256), and of the grant of the President of the Russian Federation No. MK-413.2017.1.

Interaction of the stream of the striking elements with barriers and cumulative ammunition

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Results of numerical modeling of interaction of a stream of the striking elements with the spaced barriers and cumulative ammunition are presented. Modeling is carried out in three-dimensional statement by means of the author's computing code EFES. Range of speeds of interaction 0.6–3 km/s, and angles of a meeting from 0 to 60° is considered. Influence of speed of impact, a form of the striking elements on destruction of designs is investigated. Comparison with experimental data is carried out.

The work has been conducted with the financial support of Russian Foundation for Basic Research (project No. 16-31-00125; project No. 16-38-00256), and of the grant of the President of the Russian Federation No. MK-413.2017.1.

Three-dimensional simulations of the impact of intensive directed energy flows on the substances

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The work is devoted to the development of the authors software package Turbulence Problem Solver [1] originally created for the investigation of three-dimensional problems of hydrodynamic instabilities. Mathematical model is based on the three-dimensional multicomponent Euler equations, the numerical scheme on the grid-characteristics scheme of the second approximation order. The functionality of the mathematical models and the numerical schemes of the package are extended to consider intensive directed energies flows. The detailed description of the proposed numerical approach on the example of the problem of high-speed impact of two metal plates [2] is presented. The problem is solved using stiffened gas equation of state with the parameters calibrated using the data obtained with the use of wide-range equations of states for the metals. All the main features of the process are discussed, namely the formation of two shock waves in the samples, their propagation and interaction with free boundaries of the samples with the formation of rarefaction waves as well as the complex behaviour of the contact surface between the metals.

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[2] Yakovlev I V 1973 *Fizika goreniiy i vzryva* **9** 447–452

Designing of two-stage light gas gun to research into shock-compressed materials

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Research of dynamic properties of structural materials one of the main spheres of development of contemporary science. Shock wave is the main instrument of investigate dynamic properties of structural materials starting from the middle of the previos century till today. Using shock wave as an instrument of research allows us to investigate compressibility of structural materials, detect phase transformations, and research into the number of other phenomena taking place in the region of high pressures and temperatures. Light gas guns and shock-wave explosion generators are commonly used for shock-wave loadung. Indisputable advantages of light gas guns are fine adjusment of impact velocity, minimum and controlled angle of the striker tilt with respect to the sample plane in each separate experiment, high homogeneity of the region of 1D flow behind the shock-wave front in the specimen under consideration. It is also important that, when measuring shock compression, the striker being accelerated in light gas gun does not get hated. The paper gives the description of two-stage light gas intended for research into shock-compressed materials properties. Technologies, the light gas gun is based on, have been previously tested in the course of specially conducted tests. The results of sasmple loading given by electrocontact and piezoresistive sensors are provided.

Optimal shape of the striker when jetless hypervelocity impact

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A hypervelocity impact with a rigid wall of a axisymmetric striker generating converging to the axis of symmetry shock wave (SW) is considered. An efficient method is proposed for calculation of the optimum shape of the striker and the corresponding optimal jetless flux, so that during all the interaction time the velocity of SW and velocity of movement of the beginning of contact of the striker with the rigid wall are equal. This realizes the so-called strong solution for the shock wave. In the example shown, the shape of the projectile is closed to conical, but unlike a cone the angle between the normal to the surface and the axis of symmetry decreases when moving from the periphery to the center.

Modeling of shock-induced ejecta from layer of spherical particles

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According to the data obtained by the photonic Doppler velocimetry (PDV) [1] shock wave propagation through a layer of bulked metallic particles produces dust ejecta consisting of fragments with various velocities. While velocity distribution of dust particles can be measured by the PDV, the spatial mass distribution and size

distribution of the fragments are hard to derive from the PDV experimental data. To study the mechanism of ejecting and composition of ejected material, direct simulation of experimental conditions have been performed with the massive-parallel SPH code. We find that the cumulative jets are produced by the collisions of neighbor spheres accelerated by a shock wave. Those of jets which are able to reach free boundary leave the layer and decay with formation of many fragments. The data we acquire via direct numerical simulation of the described process is used as initial data for further investigation of dust ejecta motion in the air with the finite differences method.

[1] Prudhomme G, Mercier P and Berthe L 2014 *J. Phys.: Conf. Ser.* vol 500 p 142027

Detection of particles ejection from the roughness of the shock-loaded metals with using synchrotron radiation

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When a strong shock wave leaves a free surface of the metals, the flows of microparticles are ejections from the surface. The number

and size of particles depends on the type of metal, purity of surface treatment, shape of the incident wave, and many other factors. Most experimental studies aimed at studying the ejection of particles from the shape and size of discontinuities (notches, grooves) on the surface of metals. In this work, we detection the particle flow from a free surface of metals with the help of synchrotron radiation (SR) from the colliders VEPP-3 and VEPP-4 in the Budker Institute of Nuclear Physics (Novosibirsk). We investigated the fluxes of micro-particles from the grooves formed on the surface of copper and tin. In some experiments, the visualization of the flow of microparticles with using SR combined with the testimony of piezoelectric sensors. The resulting distribution of masses along the flow of the microparticles are in good agreement with the calculations performed in VNIIEF.

X-ray radiography method of explosive ejection diagnostic

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Many laboratories worldwide study processes of metal ejection using various recording techniques including the flash x-ray radiography method that is capable to give obvious results and to record the cloud countours and its average density along the x-ray beam. Gas-dynamic ejection experiments put special requirement to the x-ray filming. Apparatuses with the x-raying being several orders of magnitude less compared to the above-mentioned ones are currently in demand. Considering technical aspects pertinent to x-ray filming of the lowdensity metal ejecta is the investigation area of this paper [1]. Our task primarily to optimize the mode of the flash radiography in the orderwe could characterize the low-density ejecta cloud in explosive experiments. The paper describes how the x-ray diffraction technique was further improved to register the ejection process (identification of energy to be recorded, an experimental setup, and

explosionproof shields), and presents results of investigation how radiation attenuates in metals with the low thickness when the mass of the ejecta cloud is simulated.

[1] Stolbikov M Y and Smirnov V N 2017 *Phys. Usp.* **26** 465–96

Shock synthesis of non-porous samples into flat recovery ampoules

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A shock compression is used for synthesis of new materials or phase states [1]. In this method the initiating factors of synthesis are pressure and temperature, as a rule. Because of the inhomogeneity of the starting compositions and the residual porosity, the initiation of synthesis occurs in local pockets. The process develop by means of heat and mass transfer mechanisms [2]. This leads to decrease in synthesis efficiency, as a rule. In this work we attempt to address the problem of inhomogeneity through the elimination of the original porosity. The purpose of work is to create conditions for more uniform heating of the sample under shock loading. As an object for study of shock synthesis of cubic structure (γ-phase) of silicon nitride (Si_3N_4) from initial hexagonal structure was chosen. Earlier studies have been conducted for obtaining a γ-phase in recovery ampoules from mixtures of Si_3N_4 with bromide [3] and copper powder at pressures up to 50 GPa [4]. In this work experiments on receiving of γ-phase of silicon nitride Si_3N_4 in recovery ampoules under the pressures of 52–98 GPa by means of explosive lenses and flat drummers, dispersed to different velocities are made. Powder Si_3N_4 with hexagonal structure was pressed in several stages into the ampoule with flat geometry. The residual porosity of the dry sample has reached 43%. Impregnation of the sample with liquid bromoform ($CHBr_3$) ensured the elimination of the pores.

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[2] Grover R 1974 *J.Appl.Phys* **45** 146
[3] Yakushev V and et al 2015 *Combust., Explos. Shock Waves* **51** 603–610
[4] Yunoshev A 2004 *Combust., Explos. Shock Waves* **40** 370–373

Burning of powder mixture Al–CuO under initiation of reaction by a shock wave

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Experimental data on initiation by the shock wave of chemical interaction between copper oxide and aluminum are described. Powders of starting components had mixed in stoichiometric ratio and had subjected to mechanical activation in a ball mill. Then mixture was compacted into the tablets 8 mm in diameter for tests. The initiation of chemical reaction between components of a tablet by shock impact had carried out inside the steel tube through the steel piston during detonation of the explosive charge. Explosive charges had a mass of 1 g with density of 1.15 g/cm^3 in all cases. The masses ratio of the explosive charge, of the piston and of the tablet were kept as 1 : 1 : 1 always. Experiments have allowed to establish that shock load and the subsequent unloading are causing dispersion of the tablet on the reacting and not-reacting clusters of components. On a cut of a steel tube all clusters are accelerating in waves of unloading. Random distribution by mass of clusters sets for them the different velocities, that leads to formation of an expanding stream of the accelerated clusters. The further process of chemical transformation occurs outside a tube with formation of expanding area of a luminous flame. Expansion in the longitudinal direction occurs with an initial velocity of 800 m/s. Diametral expansion of area occurs due by side-unload of the stream body with a velocity of 200 m/s. A relay-race initiation transfer of reaction inside not-reacting flying clusters determines the duration of combustion of a material of a tablet not less than of 5 ms. Measurement of conductivity in

the area of an illumination and review of traces on the tapes have shown presence of rarefied plasma of products of reaction along with a plenty macro-, micro- and nanoparticles.

Ignition temperature as a criterion for evaluating the reactivity of mechanoactivated composites

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For more than 15 years at the ICP RAS, the studies of detonation of mechanoactivated compounds have been carried out. The results obtained for mechanoactivated AP-Al mixtures demonstrated increasing of their detonability [1, 2]. The present report is devoted to the determination of the ignition temperature Tign as a criterion of the reactivity for different perspective mechanoactivated composites. In order to measure the flash point, the tested sample was poured on the thick copper plate previously heated to a given temperature and situated in the muffle oven. The ignition temperature was determined as the minimum temperature at which the flash of the tested sample can be observed. In so doing, the temperatures measured for HMX correlated with the data [3]. Data were obtained for AP-Al (80/20 mass) composites containing aluminium of different dispersivity. Minimal ignition temperature corresponds to the activation mode found to be optimum for detonation of loose-packed micron-sized AP-Al composites [2]. The presented technique can be considered as an express-method for determination of the optimum mechanoactivation mode.

Diagnostics of high-speed processes

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Physics dealing with extreme states of matter has finally developed into a separate scientific discipline by the middle of the 20^{th} century due to the development of the nuclear weapon where in shock waves serve as a trigger mechanism for the chain reaction. And conversely, development of nuclear charges gave an impetus to the study of physical processes observed in conditions previously unattainable in laboratory experiments. Great many phenomena and processes of the high-pressure physics is the focus of scientists at the Russian Federal Nuclear Center–Zababakhin All-Russia Research Institute of Technical Physics. The paper reviews diagnostic techniques for high-speed processes and also matter loading methods and shock-wave process registration methods used at RFNC-VNIITF to study physics of explosion and physics dealing with extremal states of matter. Shock waves are the basic tool of generating these extreme states. RFNC-VNIITF uses explosive measurement devices and loading gun-type devices to generate shock-waves and up-to-date dynamic methods to record extreme states of matter. These methods are based on different physical phenomena and principles and measure kinematic and thermodynamical parameters of matter.

Radio interferometry of shock-wave and detonation processes

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Meaningful progress can be reached in studying fast processes by implementation of noninvasive methods. Most advanced are remote interferometric methods without flow distortion, particularly, laser interferometry and radio interferometry. Radio interferometry to study shock-wave and detonation processes is applied at RFNC-VNIITF from the mid 1980s of the past age. Radiowave diagnostic method offers some significant advantages as compared to other experimental methods. The most important advantage of this method is its capability of continuous recording the motion of shock and detonation waves in optically-opaque materials, among which are almost all solid explosives (HE) and non-metallic structural materials. In some cases the radiowave method can replace at once several measuring techniques, increasing essentially the informativeness of investigations. The paper presents experimental setup to study dynamic compressibility of radiotransparent materials, including HE, and also methods to identify parameters of an equation of state for explosion products using the radiowave method. Main factors, which affect shock wave transition to detonation wave in HE were identified by radiointerferometry. HE-driven throwing of impactors and shells is studied and results of this study are given. High sensitivity of radiointerferometry to motion of different interfaces, researchability in optically-opaque media, as well as continuity of obtained data allow much room for experimental studies.

Electromagnetic technique of research into shock-wave and detonation processes

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Electromagnetic technique is a method that allow mass velocity profiles to be measured. The method, compared to the methods using integrated sensors, has the number of advantages. The time resolution, about 10–20 ns, is several times higher than the one of piezoresistive pressure sensors. Absence of hysteresis significantly simplifies results interpretation while loading considered materials with transient (time-varying) shock or detonation wave with negative-going profile. The usage of multichannel electromagnetic sensors allows us to reach high spatial resolution, which is of great importance for transient (changing in space and time) processes. In RFNC-VNIITF we use multichannel technique to register mass velocity profiles, where the field is generated with Helmholtz coils. The use of Helmholtz coils with pulse generation of magnetic field allows us to conduct research into mass velocity profiles evolution with the help of fairly simple experimental devices, without some specific requirements to electromagnet protection and climate conditions, and almost without limitation on size of tested energy-saturated material samples. The paper gives the results of the research into shock-wave and detonation processes using multichannel electromagnetic sensors. The electromagnetic technique proved itself to be very informative and good for studying dynamic properties of structural materials.

Combined use of optical analyzer technique and multiply photon Doppler velocimetry to measure the sound velocities in shock-compressed metals

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Papers [1, 2] propose to combine the optical analyzer technique and multiply photon Doppler velocimetry in every explosive experiment in order to overcome the discrepancy in sound velocities measured in shocked metals using different techniques. Efficiency of this combination is demonstrated in explosive experiments with stepped samples from the 12Kh18N10T austenite stainless steel and Mg95 grade high-purity magnesium under shock-wave loading within $\sigma_{xx} = 60$–120 GPa and 20–30 GPa, respectively. So, combined use of these techniques seriously expands their application range and reduces the number of required explosive experiments involving toxic materials. The most important thing is that this technical approach enhances reliability of recorded consistent data on sound velocities in shocked structural materials.

[1] Kozlov E, Pankratov D, Kuchko D, Ral'nikov M, Poptsov A and Yakunin A 2014 On combining the optical analyzer and laser heterodyne techniques for measuring sound velocities in shock-compressed metals and alloys for verification and calibration of modern elastic-viscous-plastic models URL `http://www.vniitf.ru/images/zst/2014/Trudi/Sec4/4-58.pdf`

[2] Kozlov E A, Pankratov D G, Kuchko D P, Yakunin A K, Poptsov A G and Ral'nikov M A 2017 *Instrum. Exp. Tech.* **60** 98–106

Use of laser interferometer VISAR for the investigation of the dynamic properties of substance modeling the emulsion explosive

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Laser interferometer VISAR was applied for investigation of shock compression waves in epoxy compaunds modelling emulsion substance. The volume fraction of the glass microspheres in the epoxy compaund was 0.7. The glass microspheres diameters were of 20 to 80 μm. Powder gun with inner diameter 57 mm was used to accelerate plane impactors of the aluminum alloy. The velocity profiles of the free surface of compaund samples were obtained at the impactor velocity region of 350 to 580 m/s. Found to be the free surface velocity profiles of spheroplastic had a two waves shape [1] unlike one wave shape in the homogeneous conpaund. The dependence of velocity rase time of free surface versus impactor velocity was obtained. The data acquired can be used for interpretation of data obtained at detonation process in emulsion explosives. The work was supported by Presidium of RAS.

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Visual analysis of quasi-detonation in porous layer

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The propagation of fast deflagration and quasi-detonations in a layer comprised of matrix of 8 mm steel cylinders has been studied experimentally using high speed self-luminous observations. It was shown that inside the pore velocity can vary from 500 up 1600 m/s, while the average velocity of quasi-detonation is 650–700 m/s. Assuming that the velocity of leading shock wave heading the reaction zone is close to the maximal velocity of reaction zone 1600 ms we can obtain the realistic value for induction zone length of quasi-detonation correlating with the size of the pore.

Non-classical detonation regimes of liquid high explosives

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To date there are a lot of data about the detonation waves structure that cannot be explained within the framework of the classical model. For example, in some pressed high explosives (HE) an increase in pressure in the reaction zone was observed instead of the Von Neumann spike. The aim of this work is the proof of the existence of a similar detonation waves in liquid HE. As objects of study selected liquid HE (nitromethane, tetranitromethane, and bis-(2-fluoro-2.2-dinitrobutyl)-formal (FEFO)) and their mixtures with

not detonating liquids (methanol, nitrobenzene and diethylenetriamine). Recording the structure of the reaction zone was carried out by the interferometer VISAR. As a result of experiments the following results were obtained. In nitromethane in the reaction zone Von Neumann spike is formed. In a mixture of nitromethane–diethylenetriamine clearly pronounced Von Neumann spike virtually nonexistent. In the reaction zone of tetranitromethane, as in nitromethane, the flow corresponds to the classical model of detonation. However, the situation fundamentally changes when you add methanol or nitrobenzene. In the compositions close to the solutions with zero oxygen balance Von Neumann spike disappears. In FEFO, there is partial decomposition of HE in front of the shock wave. Addition of methanol or nitrobenzene, in this case, reduce the rate of chemical reactions and reduce the fraction of HE reacted in front. The results showed thus that non-classical detonation regimes do not represent an exceptional phenomenon. They are observed in experiments not only with pressed (heterogeneous), but with a liquid (homogeneous) HE. The study was financially supported by the Russian Foundation for Basic Research, project No. 16-29-01002.

The formation features of a cylindrical detonation wave with a multipoint initiation

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This work is the extension of the previous works. The experimental results showing the formation features of the cylindrical detonation wave with a multipoint initiation are presented in this work. One of the main features of the process is the presence of the nodes on the detonation wave, i.e. points of convergence of detonation waves from the neighbor points of initiation. The other feature is the presence of the wisps which are exeunt to the detonation

products. The nodes are the points with high energy level at detonation front. They may cause hydrodynamic instabilities during the compression of a metal liner. The parietal flows in the cell structure of detonation products may be reason for the formation of the wisps. It should be noted that the detonation wave is always convex between the neighbor nodes, although in the initial moment the triple-wave Mach configuration is forming and it should lead to aligning of cylindrical wave. The experiments with the use of the high explosives with the different densities (from 0.95 to 1.65 g/cm^3) were carried out on the laboratory installation. The characteristic features of the detonation wave formed by the multipoint initiation can be seen both in the solid and in the liquid high explosives. Different design features (interlayers made of different materials etc.) did not lead to disappearing of wisp and smoothing of nodes at the detonation wave. This work was supported by the program of the Presidium of the Russian Academy of Sciences "Thermal physics of high energy density". The work was carried out on the equipment of Interregional Explosive Center for Collective Use.

Experimental investigation of the instability of detonation waves in liquid high explosive

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Experimental investigation of unstable detonation front structure in mixtures of liquid high explosives (bis-(2-fluor-2.2-dinitroethyl)-formal (FEFO) and nitromethane) with inert diluents (acetone, methanol, diethylene triamine (DETA)) has been carried out. Inhomogeneities have been registered by electro-optical camera NANOGATE 4BP allowing to make 4 frames with the exposure time 10 ns. According to experimental results the detonation front in

nitromethane-acetone mixture is unstable. It is evident that pulsations on detonation front do not form spatial periodic structure and their dimensions differ several times. But mean longitudinal size of pulsation is about 500 μm at 20% of acetone concentration. This means that the typical size of cell equals to reaction zone width. The same structure of cellular front have been registered in 70/30 FEFO-methanol mixture. Second kind of instability, failure waves, was observed in neat nitromethane at the free surface. In this case the stability loss result in turbulent flow which is clearly detected in the shots obtained. Adding small amount of DETA (0.5%) results in disappearance of the failure waves and flow stabilization. The effect is caused by the fact that DETA sharply accelerates initial rate of chemical reaction because it is sensitizer for nitromethane.
The research has executed for the project Russian Foundation for Basic Research No. 15-03-07830.

Structure of detonation waves in the case of sound velocity change in the detonation products

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As is known, there is a self-sustaining supersonic stationary wave with energy release (in the case of reactive mixtures). This is Chapman-Jouget (CJ) detonation regime. In the idealized one-dimensional formulation CJ detonation is considered as a complex consisting of the leading shock wave, the reaction zone (RZ) behind it and CJ plane. The plane of the CJ is a surface on which the fluid velocity is equal to the local sound velocity. There is a transition from subsonic flow to supersonic one in this plane. Equality between the flow velocity and the local sound velocity does not allow to penetrate disturbance into RZ and affect on the propagation of CJ detonation. In this paper a different mechanism of additional sound plane formation was considered for an ideal gas with variable heat

capacity. The following situation was considered: an abrupt change in the heat capacity of an ideal gas takes place behind CJ plane, that is the reason of the abrupt change of sound velocity. In this case, a new subsonic flow region in the detonation products may reappear. And a new transition from the subsonic flow to supersonic flow will produce a new (second) sound plane. Using this assumption the problem of existence of stationary detonation wave with two sound planes has been solved analytically. A criterion for the existence of such a structure was obtained. The quantitative estimation of parameters in the second sonic plane was carried out using realistic quantitative parameters.

Detonation wave structure in plasticized PETN according to laser-interferometric measurements

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In 1981-83, L V Altshuler and G S Doronin with their colleagues observed the mode of undercompressed (weak) detonation in phlegmatized explosive compositions. A specific feature of this mode is the self-similar expanding region of the steady-state flow behind the near-front peak of the pressure and mass velocity. The focus of this effort is studying mode details. The VISAR technique and the laser-heterodyne technique (PDV-technique) was used to study the plasticized PETN with the 15% content of inert plasticizer. Explosive composition charges were 60 mm in diameter and 10, 20, 30, 60, and 120 mm in length. The "explosive composition–lithium fluoride (LiF)" interface velocity was recorded at the time by exit of the plane detonation wave.

Investigation detonation failure behind the shock front in plastic explosives using synchrotron radiation

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In this work, for the study of the interaction of the detonation and shock waves were applied the fast processes diagnostics method using synchrotron radiation at the accelerator VEPP 3 (BINP SB RAS).
Interaction of the waves was investigated in flat thin layers of plastic PETN based explosives in a massive plexiglass shell. The layer of the test explosive was loaded by the oblique shock wave, which was followed by the detonation wave in the same direction along the layer. The time interval between the arrival of the shock wave and the accompanying detonation wondered assembly geometry within a few microseconds.
Depending on the interval between the waves, we have registered as undisturbed detonation wave and its failure behind the shock front.
This work was supported by the Russian Foundation for Basic Research (grant No. 16-29-01050).

The chemical composition of detonation products of condensed explosives and the electric conductivity value

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The nature of the high electric conductivity at the detonation of condensed explosives at the moment is not fully investigated. Several possible conductivity mechanisms were considered so far: chemical ionization, thermal emission, thermal ionization, the electron conductivity, ionic mechanism, ionization of water, the contact mechanism. However, none of them have become a hypothesis of the predictive power.

In recent years, the experimental data of the electric properties obtained for the different explosives with very varyous initial conditions and detonation characteristics. It is possible to make conclusions about the key factors responsible for the high electric conductivity at the detonation of explosives. In this paper, for the first time were considered in details the correlation between the electrical conductivity and the composition of detonation products at the Chapman-Jouget, which accounts for more than 97% by weight: CO, CO_2, N_2, H_2O, condensed carbon C. In the work was used the experimental data for the different initial density of five explosive (PETN, HMX, RDX, TNT, TATB) and the results of the calculation using the BKW modified equation [1]. It has been shown that the electric conductivity is related with the carbon content.

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Morphological and spectral analysis combustion product of aerosuspension aluminum boride nano-particles

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The aim of this work is the study of condensed and gaseous products of combustion aerosuspension nano-dispersed particles of aluminum borides (BA) using electron microscopy and recording the emission spectrum in the visible wavelength range. Nano-particles obtained by the developed RSI CTOC technology. The particles specific surface is $S_{\text{sp}} = 19.1$ m^2/g. The condensed combustion products are formed and collected after the flame propagation process aerosuspension aluminum boride particles. The working section is equipped with front wall of the PMMA, which allows to register using a spectrograph ISP-51 BA-flame spectrum. Transparent elements allowed to register during the propagation of flame green color, indicating the presence BO_2—molecular bands in the wavelength of 547 nm. Due to the gravity of the combustion products and unburned particles BA clung to the bottom cover of the working area. Selected samples were analyzed on a Philips electron microscope. Particle images indicate that in the process of flame propagation and chemical reactions on the surface of BA formation of spherical particles is the particle diameter below 100 nm, which may indicate the formation of aluminum or boron compounds. This is confirmed by the results of the elemental analysis using a microprobe Edax-32 showing the content of free aluminum and boron in the different samples. This work was supported by President grant for leading scientific schools of Russia, project NSh-9774.2016.8.

Initiation of the nitromethane by exploding wires

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Experiments have been carried out on initiation of liquid high explosives (LHE) by an electrical explosion of wire array. Experimental setup includs high voltage RLC-circuit, thin-wall plastic vessel with LHE and exploding wires. Nitromethane-DETA mixtures have been investigated at different conditions of initiation. Low sensitivity of the mixtures demands a sufficient size of the initiation spot and high enough pressure. Irrespective to power of an initial pulse, the non monotonic evolution of high energetic process could be observed, as well as failure of a detonation. At a low pulse of pressure, the total amount of output heat would appear sufficient for conventional LHE burning. In addition, experiments will be interesting with Al-Cu foils specimens in the given scheme, to measure amplitudes and profiles of waves of pressures.

Atomistic simulation of hotspots in model energetic material

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Hotspots [1] created in the center of cylindrical sample up to the temperature, high enough to run exothermal reactions for tens of picoseconds, are simulated via molecular dynamics (MD) in AB

energetic material [2]. A classification of hotspots with different time characteristics is proposed.
A single hotspot (HS) is made using quick heating so that acoustic time of the material within HS has a greater magnitude. The size of heated domain defines a time before the rarefaction wave comes to the center of HS. A critical radius of the HS in the simulation corresponds to the equality of characteristic time of isochoric thermal decomposition and the acoustic time. Decreasing radius of the HS lead to the earlier arrival of a rarefaction wave. A HS in a mechanical equilibrium of hot and cold media is simulated. Preparation of the HS in MD simulation employs two thermostats: high temperature thermostat within the HS and low temperature in the rest. Another case, which simulated in MD, is a hotspot from symmetrical collapse of a cylindrical pore which is cut out from the sample of AB material. The sample prepared initially in a state taken from shock Hugoniot. An increased concentration of free atoms A and B (radicals), which appears during the collapse, results in faster reactions in the center of such HS.

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Mechanism of plasma-assisted ignition for H_2 and C_1–C_5 hydrocarbons

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Nonequilibrium plasma demonstrates ability to control ultra-lean, ultra-fast, low-temperature flames and appears to be an extremely promising technology for a wide range of applications, including

aviation gas turbine engines, piston engines, ramjets, scramjets and detonation initiation for pulsed detonation engines. To use nonequilibrium plasma for ignition and combustion in real energetic systems, one must understand the mechanisms of plasma-assisted ignition and combustion and be able to numerically simulate the discharge and combustion processes under various conditions. Numerical simulations of the discharge processes are generally based on the solution of the Boltzmann equation for electrons and on the balanced equations for the active particles. The input data are electron-molecule cross sections and the rate constants for reactions with excited and charged particles. These data are available for simple molecules such as N_2, O_2, H_2, and, to a smaller extent, for simple hydrocarbons till C_5. A new, validated mechanism for high-temperature hydrocarbon plasma assisted combustion based on these data was built and allows to qualitatively describing plasma-assisted combustion close and above the self-ignition threshold. The principal mechanisms of plasma-assisted ignition and combustion have been established and validated for a wide range of plasma and gas parameters. These results provide a basis for improving various energy-conversion combustion systems, from automobile to aircraft engines, using nonequilibrium plasma methods.

Autoignition of n-decane–air mixture at high-to-intermediate temperatures

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A rapid compression machine has been employed to study ignition of stoichiometric n-decane–air mixtures at pressures 0.6–1 MPa and temperatures 820–900 K in order to sew new data with the high temperature shock tube measurements [1]. The high-speed imaging of ignition process was performed because the unavoidable presence of contaminating ultrafine particles, as well as their capability to be auto-ignited and to provoke ignition of gas mixtures has been

found previously [2]. In current study volumetric and insensitive to burning particles ignition of n-decane was observed. The significant difference of ignition delay times from multiple runs under identical conditions was found. The light emission observation showed that more rapid ignition can be attributed to low-intensity light appeared in the combustion chamber at different time moments. Due to sensitivity limitation of CCD sensor of the high-speed camera, the source of this light was not established. The longest of ignition times measured from repeated runs were selected as representative data and compared with the reported literature data. Current data are well jointed with shock tube data for the similar mixture density and together exhibit a monotonically increasing trend of ignition delay with a decrease in temperature. No evidence of the onset of the NTC-like behavior for ignition delay n-decane–air mixture is seen for studied conditions.

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Shadow diagnostics of hypersonic flow (M = 18) over sharp cone

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This paper presents the results on obtaining the hypersonic flow of short duration, the shadow flow visualization over sharp cone with 12° half-angle and a zero angle of attack, as well as the determination of Mach number on the cone by the shock wave angle. The use of light-gas gun, in which instead of the accelerating channel with projectile installed Laval nozzle, provides a hypersonic flow with a high optical density of the outflowing gas. Experiments was conducted in a vacuum chamber at a residual gas pressure of 1 Torr,

light-gas section was filled with helium up to a pressure 40 bar. The piston, which causes adiabatic compression of light gas, was set in motion as a result of erosion magneto-plasma accelerator discharge (capacitor bank of 1200 μF charged up to 4.5 kV). Just before the convergent part of the Laval nozzle was installed a set of brass diaphragms. Diaphragm rupture occurred at a pressure of about 1600 bar. Cone was fixed firmly coaxially with the nozzle at a distance of 20 mm from the edge a nuzzle. Registration of shadowgraphs was carried out using high-speed camera Photron Fastcam with an exposure time of 1 ms and speed 300,000 frames/s. To visualize the hypersonic flow over the cone a knife and slit shadow method was used.The halogen lamp was used as a light source. Calculation of the Mach number was based on measurements of the shock wave angle on the shadowgraph. The obtained value of M = 18 for a cone with half-angle of 12° corresponds to the maximum value of incident flow. Further on the density distribution across the flow field was calculated procceding shadowgraphs by use of Abel equations,since the streamlined body has an axis of symmetry.

Instability of a planar detonation wave

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The paper is devoted to the numerical analysis of planar detonation which according to the classical theory represents a self-sustained propagating reaction wave coupled with a shock. Detailed theoretical analysis predicts the instability of such a structure due to the finite thickness of the induction zone between the leading shock and the zone of exothermal reaction. Different modes of oscillations of detonation parameters could be observed depending on the numerical method features and initial conditions. Properties of these oscillations in hydrogen–oxidizer mixtures are obtained with use of

contemporary dissipation free numerical methods. Obtained results allowed defining resonant wavelength corresponding to the characteristic scale of planar detonation oscillations which can be used to determine physical connection between one-dimensional detonation instability and multidimensional detonation cells structures.

Decaying modes of spinning detonation in narrow channel

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Typically, a propagation of detonation in subcritical narrow channels is accompanied by spinning or galloping modes of propagation. These phenomena are due to the intense heat transfer from a reaction zone to the walls, as well as an interaction of the shock front and the reaction zone with a boundary layer. Transition from the diagonal forms of propagation to the spinning ones in rectangular channels are of particular interest [1–3].

The present work is devoted to a series of experimental investigations of the decaying spinning mode of the flame front in the long (1000 mm) channels of subcritical diameter (3 mm), when the velocity was significantly lower than the velocity of the stationary Chapman–Jouguet detonation. The aim of the work was to determine the dynamics and concentration limits for the decaying spinning flame propagation in acetylene–air mixture. The streak images were obtained using the high-speed camera "Videosprint". Dynamic parameters of the damped shock wave were determined using pressure sensors by PCB. The pressure on the front of the shock wave dropped by 10 times. Time delays between the shock wave and the reaction front were measured. The characteristic delay was 200 μs. The spinning mode of the propagation was detected for equivalence ration of 0.9–1.6.

This work was supported by the Russian Foundation for Basic Research grant No. 15-38-70017, 16-38-00682 and grant of President of the Russian Federation No. SP-1501.2016.1.

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Flame front propagation during a detonation decay in tubes with porous coating

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Ensuring the safety of the production and storage of hydrogen is one of the most important tasks in the field of hydrogen energy. Since the detonation wave has a cellular structure, one way to prevent the detonation is to use the porous coating to reduce the intensity of transverse perturbations [1, 2]. The aim of this work was to study flame propagation and shock wave dynamics in a channel with porous walls: steel wool and polyurethane foam; and to compare the detonation parameters in channels with solid walls. Mixtures of hydrogen with air have been used with different concentrations of hydrogen. In all mixtures the detonation wave was formed before reaching the section with a porous coating.

In both porous materials, the stationary detonation wave decoupled in the porous section of the channel into the shock wave and the flame front with velocity around the Chapman–Jouguet acoustic velocity. The pressure peak by the end of the porous section with steel wool and polyurethane foam was 10 and 6 times lower, respectively, than in the channel with solid walls. The flame velocity dropped below Chapman–Jouguet acoustic speed in both cases and was 25% lower in the case of steel wool. Deviation from a stoichiometric mixture resulted in stronger detonation attenuation. Significant shock wave curvature by the end of the porous section was found when using porous materials.

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

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Express-method of evaluation of heat losses behind a front of decaying detonation wave under a metallic porous surface

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One of the important problem of ensuring safety is the problem of prevention of the explosion in gas mixtures. Often the most dangerous is associated with a detonation combustion with a sharp increase in pressure up to several tens of atmospheres. The subject of investigation was to determine a heat loss, which results at using the metallic fiber coating, as well as the determination of effective heat-conducting layer of the metal porous surface.
A numerical method is suggested for rapid evaluation of heat loss in a narrow boundary layer of a channel behind the front of the detonation wave. Channel with solid walls is under consideration, the inner surface of which is covered with a porous thin layer. The layer consists of a metallic "wool", is that of a layer of woven metal fibers. A separate isolated iron fiber having a diameter of 30 μs was considered. The calculation of the heat flow was carried out numerically using an explicit scheme in axially symmetric setting.
Full heating metal fibers occurs at times of order 10 μs. On the basis of comparison with the overall heat losses, estimated in a track hot products, an effective heat-conducting layer of the metal porous coating was determined. The specified thickness of the order of 0.4 mm and a porosity of 0.998 degree coverage.

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Influence of hydrogen–air mixture composition on the development of spherical detonation under direct initiation

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The formation of detonation in the gas mixtures are always of great interest to researchers. A particular place in theory occupies the detonation in the spherical flames, because as opposed to flames in tubes the walls does not influence on the development of the process. After the events at a number of nuclear power plants (Chernobyl, Three Mile Island, Fukushima) this is also acquired the great practical interest, since during an accident at the nuclear power plants large amounts of hydrogen–air mixtures are generated. For development of the spherical detonation of hydrogen–air mixtures even at direct initiation it is required mixture volume of several cubic meters or more. In this study, the hydrogen–air mixture was in a thin rubber envelope with volume of 7 m^3, having a shape close to spherical, which was placed in the explosion chamber 13Ya3 with inner diameter 12 m. To date in investigations of formation of detonation of hydrogen–air mixture at direct initiation only boundary curve of detonation in the chart “mixture composition–energy of initiation” was determined. This curve has the shape of a parabola. Questions as the detonation of hydrogen–air mixtures develops and at which distance from the point of initiation the detonation is determined have not been studied previously. This work is aimed at studying these questions both for the compositions on this curve and inside the region bounded by the curve. The hydrogen–air mixtures with hydrogen content from 29 to 43 vol.% at initiation energy equal

to 15.5 kJ have been investigated. This work is supported by the Russian Science Foundation (grant No. 14-50-00124).

Mitigation of explosions of hydrogen–air mixtures using bulk materials and aqueous foam

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The objective of this work was to determine experimentally the effectiveness of protective barriers when the blast action occurs as a result of premixed hydrogen–air combustion in various regimes. Experiments were conducted in a vertical shock tube having a diameter of 54 mm and a length of up to 2 m. Blast loads were created by using ring obstacles to accelerate premixed hydrogen–air flames. Comparative tests were performed of bulk materials with different densities and aqueous foams with different expansion ratios. It is demonstrated that the degree of blast attenuation using aqueous foam increases with decreasing molecular weight of the filling gas and increasing density (decreasing expansion ratio) of the foam. A bulk Aerosil barrier three times thicker than a titanium-dioxide one is found to have a similar attenuating effect on blast action. However, the mass per unit area of an Aerosil barrier is lower than titanium dioxide by a factor of 6 and is comparable to foam. The dependence of blast attenuation on parameters of bulk materials and aqueous foam must be taken into account in the design of explosion mitigation systems for hydrogen leakage and combustion.

Pulsation regime of detonation combustion of air–methane mixture in supersonic flow

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Results of analytical description and experimental study of detonation combustion regimes of air–methane mixture in supersonic entraining stream inside the cylindrical channel are presented. A wide range of mass ratio of components and initial temperature of fuel mixture is considered. Mathematical model is proposed for prediction of propagation rate of detonation wave front confirmed the original results of experiments and empirical data of other authors. The possibility of implementing of pulsating regime of detonation combustion of air–methane mixture in supersonic flow with Mach number M = 3 is experimentally confirmed. It is observed that most steady pulsation regime is realized in range of air excess factor = 1.0–1.4. It is shown that detonation is degenerated and combustion regime of mixture becomes turbulent at temperature of air flow over 1650 K. Obtained data can be used in experimental studies of detonation processes, creation and testing of advanced energy and propulsion systems, bench and process equipment.

Operating process in detonation burning facility numeric simulation

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A pulse detonation engine (PDE) is considered as a perspective high-speed aircraft propulsion. PDEs are expected having some advantages in comparison with ramjets at high Mach numbers of flight, in particular, lower heat flux in combustor walls and at the same time has high thrust characteristics. The results of different operation modes of detonation burning facility (DBF) numeric research are described in the paper. This DBF simulated an operating process in the PDE's combustor. The flow passage of the DBF is a slightly divergent tube with fuel injectors in the front section and cavern in the back one for burning initiation and stabilization. Flow parameters were obtained by Favre-averaged Navier–Stokes equations for reacting air–hydrogen mixture integration. At the same time both atmosphere and high-altitude exhausts were considered. The calculations showed significant exhaust conditions influence on detonation wave initiation process. As well there is to be flow blocking in the fuel injectors at some regimes of DBF operating. The comparison of calculations results with experimental data from DBF of CIAM are also presented.

Shock tube investigation of hot points emission in shock-wave front propagating in noble gases mixtures

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The shock waves propagation in two-component mixture of noble gases was studied experimentally. The heavy gas concentration was small end free path length in paired collisions of heavy particles was a lot more path length in collisions of light particles. The study was performed in high vacuum shock tube of stainless steel with a caliber of 100 mm in the range of Mach numbers from 2.3 to 3.5. Upgraded laser schlieren method, patent No. 216.013.4412, and multichannel emission spectroscopy high resolution on the basis of ACTON 2150 spectrograph equipped by high–speed camera LeGa-2 were applied. The range of sensitivity lies in the spectral region from vacuum ultraviolet to near infrared. The profiles of density changes in front of the shock waves were measured. The local centers of superequilibrium radiation in front of the shock waves were detected. The analysis of the observed phenomena is discussed. This work has been done due to program of Presidium of RAS.

On chemical inhibition of shock wave ignition of hydrogen–oxygen mixtures

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The prevention of catastrophic explosions of hydrogen is the actual problem for existing and developing energy technologies. An introduction of chemically active inhibitors which suppress the combustion and detonation development is widely considered, but their opposite influence on ignition at certain conditions has been also reported [1].The goal of present work was the experimental study of the influence of the wide range of various inhibitors on shock-induced ignition of hydrogen. Experiments were carried out in the shock tube of standard design in the stoichiometric hydrogen–oxygen mixtures diluted with argon to 10–20% and doped with 1–3% of studied suppressants, namely CCl_4, CF_3H, $C_2F_4Br_2$, $C_3H_9O_3P$, CF_3I and C_3F_7I. The ignition delay times after the reflected shock wave propagation through the investigated cross-section were measured using the OH emission signal at wavelengths 306–310 nm. The specific values of T and P were derived from the incident shock wave velocity measured by piezoelectric pressure gauges. Modern kinetic mechanism of hydrogen combustion was used for the following modeling and analysis using ChemKin software package. Observed temperature dependencies of induction times indicates that CF_3H and $C_3H_9O_3P$ certainly lack inhibiting activity at given conditions, while the effectiveness of halogen-containing specie dramatically increases in a row Cl→Br→I. C_3F_7I provided an unique combination of combustion suppression activity and safety for human health and ecology.

This work was supported by Russian Science Foundation grant No. 14–19–00025.

[1] Drakon A and Eremin A 2017 *Comb. Flame* **176** 592–598

Methane and hydrogen ignition with ethanol admixture

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The tightening of environmental standards for the concentration of greenhouse gases and soot particles emission from the combustion of hydrocarbon fuels requires the development of new fuels. One of the most promising ways to solve this problem is the partial or complete replacement of fuel by biofuels. In particular, ethanol is widely used type of biofuels. The experiments were performed in stoichiometric mixtures of methane–oxygen and hydrogen–oxygen with additives of C_2H_5OH behind the reflected shock waves in the temperature range of $T_5 = 1000$–1825 K and pressure range of $P_5 = 4.8$–5.98 bar. The ignition delay times were measured by chemiluminescence emission of OH radicals at 306 nm and simultaneous pressure sharp increase in all investigated mixtures. It was shown that ethanol admixture to methane–oxygen blends leads to the decrease of ignition delay times. Whereas the ethanol admixture to hydrogen–oxygen blends leads to the increase of ignition delay times. Ethanol, methane and hydrogen oxidation kinetics paths in ethanol–oxygen, methane–ethanol–oxygen, hydrogen–ethanol–oxygen mixtures were analyzed. A significant difference between the existing models of ethanol oxidation was shown. The new kinetic mechanism of combustion of methane and hydrogen with admixture of ethanol was compiled from literature data for elementary reactions and validated on obtained experimental data. This work has been supported by the Russian Science Foundation, project No. 14-19-00025.

Heat effects and soot yield in shock induced pyrolysis of C_2H_2 and C_6H_6 mixtures doped with H_2, O_2 and CH_4

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This study provides temperature dependencies of soot yield in shock-induced pyrolysis of acetylene and benzene mixtures doped with H_2, O_2 and CH_4 additions. Extinction time profiles were measured in the visible (633 nm) and IR (2.7 μm). The relative soot yield at a fixed time, the induction times and the effective rate constants of carbon particle formation and were determined as main kinetic characteristics of soot growth. The temperature profiles during the induction time were recorded using a pair of tunable quantum-cascade IR diode lasers adjusted on two CO lines at 2111.54 and 2191.50 cm^{-1}. For this measurement, 0.1–0.8% CO was added as a tracer and 20% He was added as a vibrational relaxant in studied mixtures. The modeling was carried out in a software package of ChemKin and in an original package in zero-dimensional isochoric approach.

The results of experiments as well as numerical simulations have shown that the acetylene pyrolysis, particularly in presence of hydrogen, do not produce notable heat effects. An addition of oxygen, though, results in a significant heat release. The drastic drop of the measured temperature due to decomposition of initial molecules was observed in benzene. The observed shifts of temperature dependencies thus could be attributed to the thermochemistry of hydrocarbon oxidation and pyrolysis.

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Promotion of methane ignition by the laser heating of suspended nanoparticles

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The development of new methods of ignition promotion is an actual task. The influence of additions of nanoparticles on methane combustion was studied previously [1] and resulted in twofold acceleration of ignition at T <1400 K. The goal of the present study was the investigation of the impact of laser-heated nanoparticles on methane-oxygen mixture ignition. The nanoparticles were synthesized in pyrolysis of 0.5–1% $Fe(CO)_5$ and 1–2% of C_6H_6 diluted in argon in the experiment before the ignition test. The residual nanoparticles were pulled into the flow behind the shock wave and their volume fraction was measured by laser light extinction. Just after the reflected shock wave propagation particles were heated by the impulse of Nd:Yag laser. Temperatures of heated particles were estimated using laser-induced incandescence methods. Modern kinetics of methane combustion was used for the modeling and analysis.A significant decrease of ignition induction times was observed as a result of a laser impulse. Analysis performed has shown that the effect supposedly involves catalytic reactions of methane decomposition on the surface of heated particles and allowed estimating their effective activation energy. This work was supported by Russian Science Foundation grant No. 14-19-00025.

[1] Gurentsov E V 2016 *J. Phys.: Conf. Ser.* **774** 1215–1222

Excitation of acoustic oscillations arising during the combustion of aluminum particles in a channel of variable cross section

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Theoretical study of the excitation of acoustic oscillations arising during the combustion of aluminum particles in a channel of variable cross section was performed. The flow in the channel was assumed to be one-dimensional. In the transverse direction took place complete mixing. The aluminum particles were considered spherical, monodisperse and stationary relative to the gas. It was assumed that the aluminum particle combustion took place in the diffusion mode. Coefficients of the binary diffusion were considered identical and independent of the concentration of the mixture components. The Lewis number was assumed to be equal to unity. Soret and Dufour effects were considered negligibly small. It was shown that increasing the channel cross-section leads to attenuation of acoustic oscillations and vice versa. The approximate formulas for the frequencies and the increment of the acoustic oscillations were obtained.

Self-organized micro-nano-scale patterns formation and excitation of the unique set of holograms of the energetic materials reactionary zones

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The aim of this research is development of the new concept of application of the unique set of holograms of the energetic materials reactionary zones for manipulating by the resonance spectrum of the micro-nano-scale structures of the energetic materials reactionary zones. According to our hypothesis each energetic material has a unique set of holograms of the reactionary zones in available specific frequency bands. In the energetic materials reactionary zones can be observed a unique set of holograms: image hologram, acoustic (cymatic) hologram, electromagnetic hologram, thermal hologram. The analysis of available experimental data show that micro-nano-scale structures forms both the fractal and micro-cymatic patterns in the reactionary zones and can be considered as a fingerprints of the set of holograms of the reactionary zone. For practical applications in the aerospace propulsion area we suggest new technology of scanning of the multi-component unique resonance spectrum of all molecules in the reactionary zones and programmed transfer of the quantum information into the reactionary zones for excitation of the resonance spectrum of the predetermined set of molecules by means of resonance laser radiation or by use of the system of resonance electromagnetic and acoustic fields. Such excitation along with re-programming of the resonance spectrum of the micro-nano-scale structures of the reactionary zones gives the possibility for control by the scale and 3D localization of the induction and energy-releasing areas and, accordingly, allows control inter-scale interaction in the aerospace propulsion systems.

On the description of the turbulent flame acceleration with Kolmogorov law

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A series of experiments on the flame propagation in a hydrogen–air mixtures in a cylindrical envelope of 4.5 m^3 volume were carried out. Flame front propagation was recorded using ionization probes and video in the visible and infrared ranges. The dependences of the flame front position on time for various gas mixtures were obtained. The interpretation of the obtained results using the acceleration model of turbulent gaseous flames based on the Kolmogorov law [1] identified the need to adjust this model. Model of accelerating turbulent gaseous flames based on the Kolmogorov law with constant specific turbulent energy dissipation rate of a good description for the flames, accelerating according to a power law with an exponent of 1.5. However numerous experiments with different gas mixtures show flame acceleration with an exponent of 1.01 to 3 [2]. This indicates a change in the specific energy release and dissipation rates concerned with various events in the flame front, which cause both growth and reduction of specific energy release rate. Supplement of model with the possibility of changes in the specific turbulent energy dissipation rate confirms the applicability of the approach of Kolmogorov to describe the flames accelerating by a power law with an exponent different from 1.5.

The study was performed by a grant from the Russian Science Foundation (No. 14-50-00124).

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Expanding hydrogen–air flames in a cylindrical envelope

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Free spherical premixed flames propagation is studied for a long time and up to now there no agreement between different descriptions of experimental data. The aim of this investigation is propagation of hydrogen–air flames in a cylindrical envelope at the ignition close to the bottom of envelope. Combustion front behavior during hydrogen–air deflagration in cylindrical envelopes was experimentally studied using ionization gauges and infrared photography. Hydrogen–air mixtures of various concentrations were filled into the polyethylene envelope of 4.5 m^3 and ignited with exploding wire of 5 J energy.

The flame propagates after initiation hemisphericaly with a subsequent transition to quasiparallel propagation. At every stage the flame front position dependence on time was approximated with the power function. The speed of flame propagation and the power function exponent was changed abruptly at the transition from one stage to another.

For each stage of flame propagation the preexponent, Reynolds, Lewis and Peclet numbers were calculated according to the results of experiments. The dependences of the curvature of the flame front and the scale of the velocity pulsations near the front were found.

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Thermal explosion in the process of acetylene pyrolysis

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The paper studies numerically the peculiarities of non-steady evolution of the thermal explosion arising in oxygen-free compounds of acetylene based mixtures in conditions of shock compression. To obtain quantitative estimations of the explosion characteristics a semi-empiric model of acetylene pyrolysis is elaborated. The model takes into account the following elementary processes: acetylene decomposition, basic stages of polymerization, carbon particles nucleation, coagulation and surface growth. The later is modeled in approximation of hydrogen abstraction–acetylene addition (HACA) mechanism. Empirical constants are fitted using available experimental data on induction delay times and rates of condensed particles growth. As a result calculated growth of condensed phase of carbon nano particles and corresponding thermal effect agree well with experimental data obtained in shock tubes. It allows analyzing numerically the formation and propagation of reaction waves behind the reflected shock waves in shock tubes. Depending on the rate of exothermal reaction different modes of reaction waves are observed. The minimal initial speed of reaction wave corresponds to the reflected shock speed. In case of higher rates a supersonic detonation-like waves can be registered.

Flame propagation in poorly-stirred hydrogen–oxygen mixture

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The paper considers numerically the pecularities of flame propagation through the channel filled with poorly-stirred hydrogen–oxygen mixture. The stages of flame acceleration and transition to detonation are analyzed in a conventional problem setup [1, 2]. Poorly-stirred mixture is a medium in which the reactants are distributed averagely isotropically but with small-scale spatial non-uniformities. Characteristic scale of the non-uniformities is chosen to be of the order of $\delta \sim \ 0.1 - 1.0$ mm. The non-uniformities are distributed isotropically. And the reactants concentrations for each non-uniformity are dispersed according to normal law with given scatter σ. The rate of stirring is controlled by varying parameters δ and σ. Such a problem setup differs sufficiently from the problem of non-premixed combustion when the reactants are splitted spatially. It is shown that relatively small scaled non-uniformities (of the order of flame front thickness, $\delta \sim L_f < 0.5$ mm) with relatively small value of dispertion ($\sigma < 0.15$) leads to the increase in rate of flame acceleration and faster onset of a detonation compare with premixed case. Non-uniform reactants distribution determines the perturbations birth on the flame surface due to differences in combustion rates. The smaller is δ the smaller is the scales of perturbations on the flame surface and the higher is the rate of flame front instability. As a result an acceleration of the flame takes place. The larger is δ and/or σ the greater role belongs to the factor of flame decelaration or even quenching when interacting with regions containing mixture with compound far from stoichiometric one.

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[2] Ivanov M F, Kiverin A D, Klumov B A and Fortov V E 2014 *Physics-uspekhi* **57** 234–49

Influence of mixture composition and ignition timing on efficiency of spark ignition engine running on hydrogen-based mixtures

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Pressure indication was experimentally performed for spark ignition engine running on hydrogen–air and hydrogen–methane–air mixtures (90 vol.% hydrogen, 10% methane) at various air equivalence ratios from 1.5 to 3.0. Engine parameters were: 1500 rpm rotational speed, 11.4 compression ratio, 1.187 l displacement. Ignition timing when running on hydrogen–air mixtures was set 0° before top dead center (TDC). At air equivalence ratio of 1.4 and less backfire was observed. Operation regimes when running on mixtures with methane were examined at ignition timings of 0° and 2.5° before TDC. More early ignition timing led to higher values of engine working cycle characteristics: maximum pressure and indicator efficiency. The highest indicator efficiency was equal to 34% and was obtained for hydrogen–air mixture with air equivalence ratio of 1.5. Indicator efficiency in all performed experiments were in the range 27 to 34%. Two-dimensional CFD modelling of combustion in engine was performed with account of real engine parameters for hydrogen–air mixtures with air equivalence ratios in the 1.4 to 2.0 range. Theoretical values of maximum pressure turned to be less than that received in experiments that could be caused by insufficiently full description of conditions of heat transfer to cylinder walls in modelling.

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Piston engine on pure hydrogen

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Using hydrogen is considered as the most promising method energy storage. Results of experiment represented on base piston engine on pure hydrogen.Converted gas piston engine G-266 was used in experiment with pure hydrogen. Changes were included in construction engine for work on pure hydrogen. Methodology selected cylinder was used in this engine for experiment which allows explore the combustion process. The results of research are indicator diagrams at different air excess coefficient. After that calculation was produced all the basic parameters of the combustion process: Indicating pressure, power and efficiency. These results allow us to following conclusions: power control is provided through composition change mixture without breaches combustion process. In the future results will be used in test with full-size gas piston engine and in test where this gas piston engine will be used as backup power source.Research was supported by leading science school SS-8406.2016.8

Laser-induced breakdown ignition of natural gas in a 2-stroke engine

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Laser-induced ignition for internal combustion engines is investigated intensively after demonstration of a compact “laser plug”. Laser spark benefits as compared to traditional spark plugs are:

higher compression rate and possibility of almost any fuel ignition, so lean mixtures burning with lower temperatures could reduce harmful exhausts (NOx, CH, etc.). No need in electrode and possibility for multi-point, linear or circular ignition can make combustion even more effective. Laser induced combustion wave appears faster and is more stable in time, than electric one, so can be used also for ramjets, chemical thrusters, and gas turbines. Laser ignition takes place due to gas breakdown followed by plasma and shock wave formation, those lead to deflagration core onset (detonation and autocatalytic reaction are also possible). We have tested methane and isobutene–propane mix for our 2-stroke model engine. DPSS laser pulses (1064 nm, 12 ns, 30 mJ) were synchronized to top dead center for up to 100 Hz. Ignition possibility has been checked in a broad range of air/fuel ratios. Combustion brightness temperature measured was up to 2600 K, and peak pressure reached 45 bar (at 16 bar compression). Indicated horsepower was ∼15% greater than specified for gasoline, that is slightly higher than known for gas fed 4-stroke engines. NO_x concentration in exhaust 16 ppm was measured, that is significantly lower than traditional automotive engines have. Soot deposits on laser spark plug protective sapphire window were ablated at beam path. Laser ignition system allows use multiple fuels in lean mixtures at higher compression ratios, so it can be used for high performance engines (e.g. for UAV) and for harmful emissions reduce from industrial power plants.

Methane–air conical flame: Experimental and numerical investigation

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Experimental investigation on conical methane–air flame was carried out by means of high-speed video-recording with ultra-violet

objective and image intensifier "LaVision" IRO, characteristics of cold jet, formed in the same nozzle as flame, was studied by means of hot-wire anemometry. Detail description of experimental setup was shown in [1]. Mean velocity and turbulent pulsations profiles were obtained for different grid solidity. For flows that corresponds to Reynolds numbers Re = 500–2000 velocity fluctuations do not exceed 0.2–0.4% (equal for all grids). With flow velocity growth up to 4 m/s turbulent intensity increases slightly up to 0.5–0.7% while in case of grid absence fluctuations under conditions of flow velocity 2 m/s are about 1.5% and for 4 m/s–3.5%. Area of stable flames (blow-off and flash-back fields) also does not show significant changes under such variations of turbulent pulsations despite of significant velocity fluctuations $(10-15\%)$ [2]. And flame flickering frequency does not depend on grid parameters. Also decrease of flame flickering frequency with the mixture equivalence ratio growth and increase with flow velocity were found. Numerical experiment was performed based on software package "Flow Vision" [3]. The geometry of computational domain was similar to the experimental setup, computational grid was consisted of about 1 mln cells.

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Study of the burning of hydrocarbon fuels in supersonic air flow

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We developed a simulation math model of the burning of hydrocarbon fuels with sufficiently detailed kunetic mechanisms that include nearly hundreds of reagents and up to a thousand of their chemical reactions.

Model combustion chambers of different configurations were numerically accessed using the simulation model. The specific impulse of a gasdynamic truct, the efficiency of fuels combustion, and the gas temperature near the combustion chambers walls were taken as criteria to evaluate the effect of different input parameters. The computations were made for gaseous fuels supplied in bulk into supersonic air flow, luquid-drop, gas-liquid and gaseous fuels supplied from shoes in the flow and from steps on the combustion chamber walls.
The computations were made for jet propellant (kerosene), diesel fuel, gasoline, propane with a small addition acetylene. The jet propulsion was taken as a baseline judging from its output performance and usability.
We evaluated an expansion angle of combustion chamber that ensures stable burning at high specific impulse and efficiency of fuels combustion.
We investigated the influence of pressure, temperature, and Mach number at the combustion chamber entry; the fuels temperature and radiation upon the burning parameters.
We determined an average diameter of particles of luquid-drop fuels, velocities of particles and their initial direction that guarantee their full flashing and further burning.

Interaction between high-enthalpy rocket exhaust streams and dropping liquid

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When launching modern heavy- and middle-lift launch vehicles intra-stream water supply and water-screen systems are often used to decrease force, thermal and acoustic loads to the launch vehicles

structural elements. The water flow in such systems is comparable to the mass flow of gases from engine nozzles.
In this paper the interaction between exhaust streams of a space rocket and dropping liquid is studied with high-performance computer simulation.
The results of computations for interaction between a nonstationary exhaust stream generated when starting a propulsion system and a droplet phase are given, the influence of a droplet phase on the structure of a stationary anisobaric stream is evaluated.

Effect of the enthalpy of hypersonic flow on separation and heat transfer near a three-dimensional compression corner

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We have performed numerical calculations of complicated three-dimensional flow pattern with local zones of high pressures and thermal fluxes near compression corner in the hypersonic flow. Experimental studies in aerodynamic tunnels permitted drawing flow schemes in separated zones in front of a compression corner and develop empirical dependences to estimate maximum heat fluxes on the surface of the three-dimensional compression corner. However, the flow pressure and enthalpy reproduced in ground conditions essentially differ from those appeared in space. A task set in the paper lies in accessing the possibility to apply the results of ground tests to real flight of a hypersonic flight vehicle in the air atmosphere. The experimental data published in [1] were taken as the basis for the study. At the first stage of research the obtained data are analyzed with a numerical method using a model of ideal gas and equilibrium air [2]. In the second stage numerical simulation is performed for the same geometrical model and Mach number,

while the flow enthalpy and pressure correspond to the real flight conditions. In the stage a model of ideal gas, equilibrium and nonequilibrium air is used. The flow patterns near the protruding element in ground and real flight conditions are analyzed. Heat fluxes assessed numerically and empirically are compared.

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[2] Gupta R N 1991 *Calculations and curve fits of thermodynamic and transport properties for equilibrium air to 30 000 K* (NASA)

Numerical simulation of a shock wave from a near-surface exploded rocket acting on a launch facility

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One of possible emergencies that happen when a Space Rocket (SR) launch, is its explosion above a Launch–Landing Facility (LF) with the formation of an intensive shock wave that breaks LF thin-walled structures of high surface area (mobile service towers).
In this article attempts to numerically simulate the propagation and interaction of a shock wave with LF elements by solving a set of Navier–Stokes equations in 3D transient formulation using a method of control volume. The geometrical model takes into account a launch table, a gas duct, a launch facility.
In the article defined the nature of dependence of overpressure on the LF surface from a height the SR lifts, and investigated the effect of a shock wave interference in an irregular-shaped LF on the shock wave pressure.

Numerical simulation of the combustion processes in the model high-velocity combustion chamber

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The paper is dedicated to the problem of a combustion chamber formation. Initial geometry of the combustion chamber was obtained from one-dimension method that based on the optimization procedure to providing the best model drag characteristics. Following calculations were preceded in the two-dimension statement. The combustion chamber integrates with an air intake and a nozzle. Two most widely spread combustion regimes were observed in the paper (high-velocity combustion and combustion in a wave structure of a pseudoshock type). Gas-dynamic flow features in each regime were researched. Main integral characteristics of combustion chamber duct were obtained. Influence of the different hydrogen-pylons arrangement on the combustion process efficiency was explored. Moreover the influence of the isolator shape on the flow pattern was demonstrated. For numerical calculation used set of computer programs FNAS 3D, developed in CIAM. This program is based on the procedure for finding time steady-state solution using Godunov S.K. numerical scheme. A full set of Favre-averaged Navier–Stokes equations for unsteady turbulent reacting flows uses in the program. To describe the combustion of hydrogen–air mixture using a Dimitrov's detailed kinetic mechanism. .

Discrete phase simulations of liquid injection, droplet breakup in two-phase flows

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For the most part of aviation engines fuel that injected into combustion chamber is in liquid state. Once injected, liquid jet is subjected to gasodynamic forces and thus undergoes primary and secondary breakup. Liquid drops evaporate and mix with air. Fuel injection efficiency is among the main factors determining aviation combustion engine performance. Fuel injection is significant scientific problem facing challenges for numerical simulations due to complexity of two-phase physics and high demand for computer resources. This is particularly important to organize efficient fuel injection systems in RAMJET due to high gas velocities and low fuel-air mixture residence time in combustor. Nowadays the aspect of liquid fuel injection in RAMJET high-speed combustion chambers is not covered well in literature because of little publications of numerical and experimental data.

Two series of simulations are performed in current study. Firstly, the simulation of liquid injection into low-velocity combustion chamber with constant cross-section area through plain-orifice atomizer are presented. Validation of numerical and physical models employed for simulation is performed based on experimental data in open publications. Numerical models are calibrated for the case of transverse liquid injection into gas flow. Secondly, the simulations of liquid injection into high-velocity combustion chamber with constant cross-section area through plain-orifice atomizer are presented. Droplet diameter distributions, evaporation rate and jet penetration depth is determined in different cross-sections.

Numerical modelling of unsteady hydrodynamic processes in serpentine type heat exchange devices

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Serpentine-type are widely used in aviation equipment and various industries–chemical, oil and gas, nuclear etc. Heat-exchange surface at that equipment is designed as flat or volumetric serpentine. Heat-transfer agent is supplied with high pressure into intertubular space. Current paper is devoted to heat exchanger design development with special requirements to thermal and stress conditions, as well as 3D-modelling of liquid flow and heat exchange processes. Conjugated heat transfer problem is modelled. In the intertubular space the turbulent flow of viscid gas with varying thermophysical properties is considered; in the tube space heat-transfer agent flow with temperature-dependent transport and thermophysical properties is considered; in the solid medium heat transfer equation with temperature-dependent heat conductivity coefficient is solved. Unsteady flow features and heat exchange features in the tube space and intertubular space are presented. Thermal transport in the solid metal body of serpent-type tubes is depicted, as well as its effect on the flow pattern. For current heat-exchanger configuration some flow regimes that provide efficient usage of heat exchanger has been determined.

Thermal and hydraulic characteristics of spherical packed beds of different configurations with real thermodynamic properties

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Porous media, formed by spherical packed beds, are presented as continuum media with equivalent hydrodynamic characteristics for the purpose of hydrodynamic and thermal calculation. Equivalent characteristics are presented by solid phase thermophysical properties, packed bed porosity and liquid phase thermophysical properties. Theoretical and experimental approaches can be used to define those parameters. The results of numerical modelling of flow and heat exchange in regular spherical packing are presented. Thermal and hydraulic characteristics with account for real thermophysical properties (including chemical reactions of dissociation and recombination on the packed bed surface) are determined. The data can be used while calculating flow and heat exchange in spherical particles porous media. The results are obtained based on elementary cell separation. Flow in elementary cell is simulated, then results are averaged and transition to continuum media properties is performed. Hydrodynamic flow pattern in porous media is obtained, then heating and cooling of spherical beds of regular geometrical packing is calculated. It is determined that in turbulent region accounting of real thermophysical properties results in 10% increase of heat transfer coefficient if compared with experimental data. It is shown that hydraulic resistant coefficient is decreased at 15% due to molecular viscosity increasing in high temperature region.

Physical and computational modeling of injecting liquid interaction with high-speed air cross-flow

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The increase of operating process effectiveness in power and propulsion systems requires the optimization of liquid fuel dispersion and mixing properties in high-speed air cross-flow. Consequently, complex calculation and experimental research can be reasonably divided into several stages: the development of multidimensional physical-mathematical model; model experiment with analogy criterion close to full-scale conditions and mathematical model specification on the grounds of experimental results; parametric computational; experimental research of a full-scale body prototype with parameters conformed to selected regimes. Experimental analysis was carried out on the laboratory test facility equipped with modern diagnostic tools such as particle image velocimetry, IMI, shadowgraphy. Model liquid dispersion characteristics in the air flow with velocity 200 m/s were obtained for swirl-type and spray injector with various geometry parameters. The specification of previously developed mathematical model of liquid drops dispersion and mixing allowed to obtain more accurate results for multiphase flow analysis.

Modeling of coupled heat-mass exchange and combustion of solid hydrocarbons gasification products and high-enthalpy air flow

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The present work is devoted to computational modeling of mixing and combustion of solid hydrocarbons gasification products and high-enthalpy air flow in the uniform cross-section channels. The coupled heat-mass exchange with regenerative cooling system is considered in the model. The main goals were the development of complex mathematical model and receiving the regularity of integral quality factors change. The methodological aspects of computation of mixing and combustion effectiveness coefficients are presented in this work. The models are based on the Favre-averaged Navier–Stokes equations for non-steady flow in accordance with turbulence. Combustion is determined by quasi-global reaction. One-dimensional mathematical model of non-steady coupled heat exchange in the cooling system is constructed with respect to longitudinal and cross-section flow non-equilibrium state in consequence of gasification products destruction. On the basis of numerical modeling analysis, the main operating and geometry parameters are obtained that correspond to effective combustion process and acceptable thermal state of the channel walls.

Numerical predictions of gauge rake thermal state in high-enthalpy flow

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It is required to have flat uniform profile of velocity, pressure, temperature and other parameters at the aerodynamic nozzle exit for correct altitude experiments on the on-ground testing rigs, imitating high Mach number flying conditions. Using special measure system with pressure and temperature gauge rake is one of the ways of controlling of flow parameters at the on-ground facility aerodynamic nozzle exit. It is well known that maximum allowable temperatures and heat fluxes depend on efficiency of water cooling of measuring rake heat-loaded parts. Thus, the main purpose of current investigation is rake parts thermal state analysis. One-dimensional calculations are not reliable enough due to complex 3D-geometry of the rake, so in current study the 3D steady-state numerical analysis is performed. At the first stage, the most heat-loaded part is analyzed and leading edge thermal state analysis is carried out, with imitation of thermal boundary conditions on coolant (water) side. Instead, convection boundary condition is applied: coolant temperature is fixed (300 K) and range of heat transfer coefficients are chosen for applied working conditions (10, 20 and 30 kW/(m^{2}K)). At the second stage the calculation of hydraulic losses in water cooling duct of measuring rake was performed in simplified approach. The approach of 2-stage numerical simulation (gas-solid domain and solid-water domain) reduced simulation time without increase of error for the current task. Efficiency of water cooling scheme in measuring system with pressure and temperature gauge rake is verified at simulation. Thus, high reliability and operability of whole measuring system is confirmed.

Problems of high-enthalpy air flow generation

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Special generators of high-enthalpy air flow (GAF) with fire heating are used at altitude testing of high-speed air breathing ramjets integrated with hypersonic flying vehicle (HFV) on ground test rigs. High-enthalpy air flow generation is realized by the way of direct combustion of fuel in oxygen enriched air. Main problems of generation underlie in aspect of imitation test rig air flow parameters maximally close to hypersonic flight condition. Key element of GAF construction is front device (FD, also called as mixing head). Fuel (e.g. methane) and oxygen enriched air are injected into combustion chamber (CC) of GAF though the FD. In CC of GAF the processes of mixing, ignition and combustion of air–fuel mixture with oxygen excess take place. Results of computation conducted with different configuration of FD shows that surface plumes and recirculation zones are formed near the FD, where the temperature is considerably higher than average total temperature in CC (up to 3000 K). Due to high temperatures, solutions at design and manufacturing are provided for avoiding FD overheating by means of installing protective cooled shield. In this paper computation investigation of hydraulic and heat characteristics in cooling cave of protective shield are presented. Necessary mass flow rate of water throw protective shield is determined for avoiding FD overheating on working regimes of GAF at flight conditions with different Mach number imitation. Altitude tests of GAF working with protective cooled shield demonstrated its workability during required time at imitation of flight conditions along HFV trajectory. Analysis of test results shown that installation of protective cooled shield provides elimination of acoustic oscillations in CC of GAF and improves combustion stability in wide range of regime parameters.

Some aspects of research object preparation for test on high-enthalpy high-altitude bench of periodic action

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Conducting research trials of experimental objects on the high-altitude high-enthalpy facilities and the stands of periodic action is a complex multifactorial and multidisciplinary task. Compliance with the conditions of flow of the research object, identical to the real requires of the free-stream parameters corresponding to the flight speed at a given height. To obtain reliable results of the research workflow in the flow path of the test object need detailed preparation, in particular pressure sensors. When vacuum (about ten mbar) and the length of pulse tube several meters settling time of the measured static pressure can reach several seconds. In a comparable duration of the specified test mode there is a risk of losing a significant part obtained from the sensor information. In addition, there is a question of interpretation of indications of the sensor, especially in conditions of unsteady processes in the combustion chamber. To reduce the delay of the measured pressure, reduce the length of the pulse tube and align the sensor as close as possible to the selection location. However, close to the place of selection pressure, the location of the sensor can lead to overheating and the inability of normal functioning. To solve the tasks proposed a new methodological approach to determine the temperature distribution along the length of the pulse tube, and then according to the results obtained for the temperature distribution to install the pressure sensor at a safe distance. In addition, the approach provides the possibility of protection as the sensor itself and its electrical connections. In the present work some results of the studies.

Developing a unique oxygen gas feed system on synthetic air high enthalpy generator of hypersonic test cell

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This report having a practical application presents a stage of calculating, engineering and experimental work series of test cell group upgrading in the research center CIAM, starting from 2008 till now by department 800 and 012. The main purpose is assuring a foreground of Russian aircraft industry in introduction of new special and certification test methods and technologies of super- and hypersonic engines and airframe. Hypersonic device researches in real flight condition are expensive and connected with fully or partial test object failure in the end of testing. Current hypersonic test cell upgrading to extend simulated real flight conditions is done by CIAM, and in spite of this the testing and research work programs are carried out, which avia- and rocket production industry offered. This work is devoted for designing a new system of storage, oxygen gas transport on plant territory and feeding on test product, flame heater and synthetic air high enthalpy generator. The system is characterized by high pressure and high oxygen flow rate values that is demanded severe requirement for reliability and operating safety. The feature of this system is that there is no analogous operated system in Russia, providing such an oxygen flow rate parameter and pressure level in balloon battery. The necessity of this work was cause of oxidant, air and fuel flow rate increase on the test cell and test product, and properly exhaust gases temperatures increase from 2000 K and more. The production project was done on basis of the results of this work. Installation of equipment is being done at this moment.

Channel geometry influence on gas-dynamic flow structure during the hydrogen combustion

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Until recently, the creation of high-speed combustion chamber for ramjet was solved mainly experimentally. However, the development of mathematical modeling currently allows to make reliable estimates of the flow characteristics of a chemically reacting mixture in the channels of different geometries, in spite of the extreme complexity of the gas-dynamic flow structure and chemical processes (even in the simplest problem of hydrogen combustion) and their interaction. The combustion chamber for scramjet was created and tested in the MAI. In this paper, the mathematical modeling of hydrogen–air mixture flow combustion was carried out and the effects of changes in the geometric parameters. Combustion and heat choke conditions at M = 2.5, T = 900 K are such that depending on the channel geometry various sonic regimes (sub-, trans- and supersonic) may be implemented.The results of mathematical modeling of gas-dynamic flow structure and the characteristics of the combustion process (heat completeness of fuel combustion) for the channel length variation with a constant cross-sectional area (with a length of changed flow regime), as well as expanding section cutout were presented. The scale factor impact (multiple change in length and height) was estimated. Calculations were performed using a set of programs designed in CIAM for two-dimensional flows with chemical reactions. It is based on the Favre-averaged Navier–Stokes equations closed by Sekundov turbulence model and the Dimitrov chemical kinetics for hydrogen combustion.

Modeling of asymmetric gas jets interaction with supersonic flow

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This work is devoted to research of gasdynamic flow properties during the injection of the asymmetric gas jets to the diverging part of a nozzle.

Numerical research of asymmetric gas jets interaction with supersonic flow is based on the multidimensional compressible Favre-averaged Navier–Stokes equations. The various models are chosen to achieve the turbulence closure. The most preferable model is k-SST because of minimal discrepancy between the obtained numerical results and other authors experimental data.

On the basis of obtained numerical results and known experimental data from BMSTU one-dimensional algorithm is developed and validated. This algorithm allows to get the characteristics of asymmetric gas jets interaction with supersonic flow in time-independent approach. It also helps to determine the direction and magnitude of a supersonic flow momentum vector at various injection parameters. The parametric research of injection impact on the gasdynamic characteristics of supersonic flow.

The obtained data are compared with the computational results of ANSYS Fluent and also with experimental data. The supersonic flow momentum magnitude in the nozzle outlet is within 5 percent error.

The developed algorithm and obtained results can be used in modern power and propulsion systems.

Simulation of ideal gas flow in the variable geometry channel with mass and energy source

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Characteristics of gas flow in the variable geometry channel with mass and energy source are studied in this paper. The channel made of energy-intensive material (EIM), capable of independent combustion, is considered. The change of geometry occurs to a specific law of EIM combustion, dependent of the local static pressure and gas flow rate. The algorithm for calculating the gas flow in a channel within the quasi-steady approach is developed to solve this problem. The solution made by finite volume method.
Algorithm based on the integration of unsteady equations system, that describes one-dimensional gas flow in a channel with distributed mass, energy and impulse source. As a result, the equations in a discrete form allows obtaining a flow field for both subsonic and supersonic flow region.
The flow at various channel configuration, the law of EIM combustion and regime parameters are investigated by using the developed algorithm. Based on numerical experiment distribution of pressure, temperature and velocity of flow along the channel is calculated and time dependent variation of the momentum in the output section is obtained.
Result can serve as an estimate of energy-power plants during design stage.

The methods for determination the influence of geometric form of turbulators on the wall flow in the supersonic stream

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Today the turbulators are widely used in the engineering technology such as aviation, jet engines, energetics. For example the turbulators are installed on the airplane wings. In this case the turbulators are stationed in the laminar boundary flow before the point of the supposing breakaway and thus help to reduce the size of separation area. This research is about the problem of using the turbulators in the supersonic stream. In particular the authors propose the methods for determination of influence of geometric form of turbulators on the wall flow in the supersonic layer. These methods are based on tridimensional numerical modeling of flow around the turbulator of given shape. The authors propose some parameters for determination the influence of turbulator on the boundary layer. These are incompressible shape factor–H and sweepout efficiency–Phi. Incompressible shape factor is ratio of displacement thickness to momentum thickness. For determination of these parameters in the computational space it is necessary to build a tridimensional platform on the sufficient distance from the turbulator. The platform settles at right angle to wall and its height is more than boundary-layer thickness delta. These values are calculated on the base of integral parameters of flow such as mass flow rate and impulse passing through this platform. This method allows to compare the turbulators of different forms and geometric sizes. This method is possible to use in cases of any sizes of boundary layer and parameters of oncoming flow.

Simulation of air cooling of supersonic testing rigs heat-loaded elements

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One of the results of aerospace industry development is movement towards higher flight speeds, which often requires the development of new or making certain changes to the existing aircraft design. It is known that fire testing is mandatory step in testing of the selected materials and aircraft schemes. For close flight condition modelling it is required to simulate incident flow parameters, what almost always means high temperature and heat flux loads on the testing rigs elements. Testing rig that is considered in the current study consists of high-enthalpy air flow generator, aerodynamic nozzle and support for aerodynamic models fixing during experiment. Many of test rig elements need active water cooling. For less heat-loaded elements air cooling is used. One of the technical realization of air cooling is directed air jet that creates air curtain and prevents surface from overheating. Interaction of two supersonic co-flow jets (air and combustion products) with temperature difference up to 1000 K. The simulation purpose is to verify operability of testing rigs elements placed behind aerodynamic nozzle exit. Two stainless steel plates are placed there and needed for support of composite elements during testing. Orifices for cooling air jets are placed at the nozzle exit. Metal plates temperature should not exceed 1000 K, while stagnation temperature of incoming gas is 1650 K. Simulation of gasodynamic is perform in steady-state approach. Radiative and convective heat transfer between support and gas is simulated. Shocks observed on the leading edge of support plates. That has negative effect on air cooling efficiency in near-wall region. Recommendations concerning air curtain cooling during experiment are given.

Flow about the tail unit of rotating arbalest bolt

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In current study simulation of flow around tail unit of rotating arbalest is performed and steady-state bolt angular velocity is determined. Tail shape provides arbalest bolt rotation and its dynamic stabilization during trajectory of flight. Initial velocity of the bolt is 110 m/s; angular velocity is up to 300 rps. It is obtained that for the simulation conditions flight range is drastically decreases if angular velocity exceed 300 m/s due to aerodynamic drag increase. If angular velocity drops to 50 rps, shooting precision is poor. Blade of tail unit has a shape of thin plate with sweep angle and a chamfer at one edge, that needed to maintain revolution, induced by side component of air drag force. Tail unit consists of four blades uniformly placed around bolt axis. Bolt diameter is 5mm and length is 700 mm. It is assumed that arbalest bolt has zero angle of attack during the flight. Numerical simulation with viscosity and turbulence effects is performed. For revolution modelling the approach with rotating reference frame (RRF) is adopted. Spalart-Allmaras turbulence model is applied. Flow pattern around rotating tail unit is obtained and air drag forces are determined. Scheme of angular velocity calculation based on moments and forces on the blade is suggested. Varying of geometrical shape of the blade is performed and shape effect on blade performance is investigated.

Diagnostics of carbon encapsulated iron nanoparticles by the pulse laser heating

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In this study the laser-induced incandescence diagnostics for sizing of carbon encapsulated iron nanoparticles has been developed.
The carbon covered iron nanoparticles were synthesized by shock waves pyrolysis of the mixtures of $Fe(CO)_5$ with C_2H_2 or C_6H_6 diluted in argon. Iron nanoparticles were formed in the shock tube behind incident shock waves at the temperatures of 700–1000 K. The pyrolysis of hydrocarbons behind the reflected shock waves at the temperatures of 1400–2000 K resulted in formation of carbon shell on iron nanoparticles. At the last stage of the carbon encapsulated iron nanoparticles formation they were heated by one pulse of Nd-YAG laser operated at wavelength 1064 nm with fluences 0.1–0.8 J/cm^2.
The LII model [1] which had been used previously for iron and carbon nanoparticles separately was updated for carbon encapsulated iron nanoparticles. Additionally, the nanoparticle samples were investigated by a transmission electron microscope (TEM). The iron core size and carbon shell thickness were measured by statistical treatment of the microphotographs. The comparison of TEM and LII particle sizing is discussed.
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The influence of methane and oxygen on carbon nanoparticle formation in acetylene pyrolysis behind shock waves

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The nanoparticles were synthesized after the heating of the mixture of 2%C_2H_2+Ar with 1%O_2 or 1%CH_4 additions behind shock waves. The conditions behind the reflected shock wave were varied in the range: $P_5 = 4$–5 bar, $T_5 = 1600$–2300 K. Particle sizing was carried out by the time-resolved four channel laser-induced incandescence method (LII), which is based on analyzing of the thermal radiation emitted by particles heated by a laser pulse. The signal decay time depends on mean particle size. The heating of particles was initiated by Nd:YAG laser pulse, at 1064 nm with fluence of 0.1–0.6 J/cm^2 and duration of 10 ns. The two-color pyrometry method was used to obtain temperature of the heated particles. Laser light extinction technique at 633 nm was used to measure the volume fraction and optical density of the condensed phase. In result of the experiments the temperature dependences of particle sizes and volume fraction of condensed phase at the last stage of particle formation were obtained. It turned out that the maximum of condensed phase yield shifts to the low temperatures with addition of oxygen and methane. The dramatic increase of condensed phase yield was observed with addition of methane whereas in pure methane the carbon particle formation is negligible in such concentrations. This study was supported by joint project DFG–RFBR (SCHU 1369/24-1; RFBR 16-58-12014).

ARAS monitoring of various halogen atoms formation in reactions of pyrolysis behind shock waves

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Atomic resonance absorption spectroscopy (ARAS) method is the most sensitive and precise method of measuring of small concentrations of atoms (in the range of 10^{10}–10^{14} cm^{-3}). This method has become a kind of "gold standard" in the study of the kinetics of dissociation of di- and polyatomic molecules.

One of the main scientific problems in combustion and detonation formation is a precise measurement of the kinetics of the most important reactions determining the influence of chemically active additives on the processes of initiating ignition of various combustible gases.

In this study a comparison of using APAC for different halogen atoms (chlorine, bromine, iodine), which are formed during the pyrolysis of the corresponding inhibitors of combustion (CCl_4, $C_2F_4Br_2$, CF_3I) behind reflected shock waves at temperatures of 1000–2000 K and pressures of 2–3 bar are presented. The paper presents the measured rate constants of the dissociation reactions these inhibitors. The experimental data can be used for the development of numerical models describing the mechanism of halogen atom formation at pyrolysis of respective inhibitors and their impact on the initial stage of the initiation of the detonation of carbon-containing compounds behind shock waves.

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Use of ARAS method for study of reaction of butanol with oxygen behind shock waves

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Biofuels, include alcohols having from 1 to 5 or even more carbon atoms are considered as the most promising types of fuel. The study of oxygen reactions with different types of biofuels is particularly important. The product of such reactions is a chain forming primary hydroxyl radical OH. However, hitherto the most rate constants of reactions between oxygen biofuels only in the low-temperature range (300–500 K) are measured. The goal of this study is the direct experimental measurements of the rate constants of biofuels reactions with oxygen at higher temperature range 900–1500 K. The time resolved oxygen atom concentration profiles the at the interaction of oxygen with butanol behind shock waves were measured by atomic resonance absorption spectroscopy (ARAS) on the line 130.5 nm at temperatures of 900–1300 K and a pressure of 2–3 bar. As an oxygen atom source for interaction reactions with butanol nitrous oxide was used, which begins dissociation on oxygen atom and nitrogen molecules already at a temperature of 900 K, where the thermal dissociation of butanol has not yet started. The temperature dependence of the rate constant of this reaction at different pressures was determined. The experimental results with the kinetic simulation using Chemkin package are compared.

The study of $C_2F_4Br_2$ dissociation kinetics using ARAS and MRAS methods behind shock waves

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Various halogenated carbons are widely used in practice for the increase of explosion safety of various hydrocarbons mixtures. Tetrafluorodibromoethane $C_2F_4Br_2$ is considered to be one of the most effective additives to the combustible mixtures, which effectively inhibits ignition and detonation processes in methane-air and hydrogen–air mixtures. However, the kinetics of decomposition of $C_2F_4Br_2$ is studied very superficially. There is an assumption that one of the secondary decomposition products is CF_2 radical, which not only inhibits the combustion under certain conditions but can even accelerate the ignition of the methane-air mixtures. Therefore, the study of dissociation kinetics of $C_2F_4Br_2$ is a very important scientific task. The study of $C_2F_4Br_2$+Ar reaction was carried out by the method of atomic and molecular resonance absorption spectroscopy (ARAS and MRAS) using resonance line of Br atom at 154.2 nm and CF_2 radical band at 251.9 nm behind shock waves. More than 40 successful experiments in the temperatures range of $900 \leq T_5 \leq 3300$ K and pressures $2.5 \leq P_5 \leq 16$ bar were performed. The initial concentration of $C_2F_4Br_2$ in argon was varied from 200 to 500 ppm. In result the time profiles of concentration of CF_2 and Br, forming at dissociation $C_2F_4B_2$ were obtained. From these experimental data the temperature dependences of the rate constants of CF_2 and Br formation and their activation energy were determined. This work has been supported by grant of Russian Science Foundation 14-19-00025.

Emission of OH^* and CO_2^* during the high-temperature oxidation of acetone in reflected shock waves

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The autoignition of a stoichiometric acetone−oxygen mixture diluted with argon was studied behind reflected shock waves in the temperature range of 1350–1810 K at the total concentration of $[M]_{50} \sim 10^{-5}$ mol/cm^3. Emission signals from electronically excited species OH^* (at $\lambda = 308$ nm) and CO_2^* (at $\lambda = 365$ and 451 nm) were recorded. It was found that the time profiles of OH^* and CO_2^* emissions reached their maxima almost simultaneously over the entire temperature range covered. It was revealed that, after reaching the maximum, CO_2^* emission signals recorded at 451 and 365 nm behaved substantially differently. Numerical simulations of the OH^* and CO_2^* emission time profiles were carried out using blocks of reactions for the formation and quenching of OH^* and CO_2^* presented in the literature. The predictions of the numerical simulation performed turned out to be in close agreement with our own measurements and the results on acetone autoignition reported in the literature.

Influence of iron pentacarbonyl additives on the formation of soot nuclei during ethylene pyrolysis behind reflected shock waves

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The formation of pure iron nanoparticles during the thermal decomposition of iron pentacarbonyl $Fe(CO)_5$, soot nanoparticles during ethylene C_2H_4 pyrolysis, and combined soot particles consisting of an iron core encapsulated into a carbon shell during the heating of a C_2H_4 + $Fe(CO)_5$ mixture in argon behind reflected shock waves is experimentally studied. The shapes and size distribution of these nanoparticles are investigated using a Zeiss Ultra Plus (Ultra 55) high-resolution field-emission scanning election microscope. Detailed kinetic simulations of the thermal decomposition of iron pentacarbonyl and condensation of iron atoms with the formation of iron nanoparticles, the nucleation of carbon (soot) particles during ethylene pyrolysis, and the process of formation of combined iron-carbon particles composed of an iron core encapsulated in a carbon shell is performed. Key parameters of the process, such as the number density of nanoparticles, their mean sizes, and their size distribution functions, are theoretically determined.

Numerical modeling of soot formation at diesel-like conditions

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The objective of this work was to use our unified kinetic model [1] for simulation of soot-forming combustion at diesel-like conditions. Resulting data were obtained at a base diesel-like operating condition, corresponding to a near top dead center compression temperature (850 K) and pressure (3.5 MPa). Data were taken for n-heptane as a "surrogate" diesel fuel in one of the fuel-rich patterns of burning jet in immediate flame proximity, where equivalence ratio ϕ was equal 3.0. Our original unified kinetic model comprises of 372 species and 4782 reactions and consists of two principal components: gas-phase chemistry of high-temperature n-heptanes' oxidation, and modified soot particle dynamics, which describes the start and evolution of the particles. The predictive power of our model was tested with injection of small amounts of H_2O_2 and H_2 additives into a rich n-heptane—air mixture patterns. These additives, as it is known, influence both the processes of ignition and soot formation. In particular, very small amounts of injected H_2O_2 enable to reduce ignition delay as well as to suppress soot formation during diesel-like combustion. The numerical simulations were validated against experimental results available in the literature. A good quantitative fit between the data calculated via the unified kinetic model and experimental data has been attained. The completed analysis might give new insights into the initial roots of soot formation process and create a magic cure for their depletion.

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Numerical investigation of initiation of gaseous mixtures containing microparticles

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At the large industrial systems such as for example coal mines or nuclear power plants there is the danger of occurring of detonation wave, which can lead to disastrous consequences.To insuring of the plant safety it is necessary to establish all possible manners/ courses of the ignition and control/ handling of them techniques. Most worrisome is detonations of mixtures of reacting gases with firm particles. The progress of the detonation initiation of combustible mixtures due to nonmoving particle is investigated. There is the only experimental work [1], which is considered to the evolution of detonation process due to additional heat generation before a particle. It does not make possible to recognize details of ignition. A two-dimensional hydrodynamic code [2] is used to simulate two-phase mixture. The code allows carrying out study of burning and combustion processes in combustible gases. Two methods of shock wave modeling are realized in the code. The wall of tube and particle are assumed to be adiabatic. Further to our preceding work [3] chemical reactions [4] are added to this one.

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The mathematical model of gas dynamics of burning aluminum diboride particles in a high-speed oxidative gas-flow

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For development of fuel compositions with a high content of metallic components it is necessary to know macrokinetic characteristics of the processes of ignition and combustion as the individual particles of powdered metals, and their complexes. The objective of this study is to simulate the processes of ignition and combustion of a single particle metallize fuel—aluminum diboride (AlB_2) in a high speed oxidative flow. The condition for complete film evaporation of the boron oxide or the condition for achieving aluminum oxide melting temperature is considered as criterion of ignition. We found the dependence of the initial values AlB_2 particle diameter and air temperature of time of ignition and combustion induction time. Calculation method which allows determining the completeness of combustion and combustion time particles in surroundings with complex chemical composition was developed for simulate the movement of reactive AlB_2 particles in a high-speed flow. The two-phase flow characteristics calculation is carried out for a fixed control volume in local thermodynamic equilibrium assumption.As a result of the numerical calculation, dependences on parameters of particles time of stay and time burn particles in the channel are obtained. Temperature field and the velocity of the gas and the dispersed phase for different times corresponding to different flow area channel are determined. This work was supported by grants of leading scientific schools of Russia project NSh-9774.2016.8.

Effect of Ce_2O_3, La_2O_3 and ZnO additives on the oxygenates conversion into liquid hydrocarbons

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A method of the waste wood processing into liquid hydrocarbons via two-stage pyrolytic conversion and the subsequent intermediate oxygenates synthesis was investigated. Synthesis gas was obtained by combination of the waste wood pyrolysis at 500–700 °C and heterogeneous cracking of volatile products in charcoal bed at 1000 °C. Additives of Ce_2O_3, La_2O_3 and ZnO have a modifying effect on the activity and selectivity of zeolite catalyst of pentasil group in the oxygenates (dimethyl ether and methanol) conversion reaction into liquid hydrocarbons. Two cases of the oxygenates processing were considered: with and without extraction from the stream of synthesis gas. The aim of this study was the efficiency test of these two cases of the oxygenates processing, selection of catalyst and the process conditions, allowing to obtain hydrocarbons with a reduced content of durene (1,2,4,5-tetramethylbenzene), that has a negative impact on the low-temperature and environmental properties of gasoline. Additive of ZnO only showed the best result: the conversion of dimethyl ether and methanol was high (81.0–88.6 and 84.0–91.0 wt.% respectively), concentration of durene in the liquid products was low (6.1–6.4 wt.%). It was also shown that conversion of oxygenates in the synthesis gas stream is stabilizes operation of zeolite catalyst and the liquid hydrocarbons have low durene content.

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Computational fluid dynamics simulations of underwater explosions

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Underwater explosions (UNDEX) refer to the detonation of explosive devices immersed in water. UNDEX present many challenges for numerical modeling. The density ratio between explosion gases and the surrounding liquid are typically of order (10^3), and the pressure ratios can be just as high. Numerical examples include verification and validation for a number of canonical test cases for two different computational fluid dynamics codes (MSC.Dytran and OpenFOAM). The first one is commercial and the second is open sourse. Shallow water explosion near a free surface was modeled and compared with experimental data obtained in NRC KI. The qualitative phenomena of bubble expansion, collapse, re-expansion and crowning are all captured by both codes. The main differences, advantages and drawbacks of the codes are shown.

Inflectional instability and large scale entrainment in free shear thermoviscous flows

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Dealing with mixing processes the viscosity is expected to play a significant role only at the micro scale rather than at the integral

one and does not have a critical influence on the large-scale entrainment. As a result, most studies investigate single-fluid or density-stratified flows. However, considering two-fluid [1] coflow shows that the kinematic viscosity variation at the interface causes multi-scale engulfment, whereas in constant-viscosity flows conventional Kelvin–Helmholtz vortices are generated. The effect of viscosity on mixing was studied experimentally [2] when turbulent low-viscosity fluid is injected into more viscous medium. Changing viscosity ratio R_ν in range of 1–400 at Reynolds number $\mathrm{Re} = 1000$ leads to significant differences in mixing evolution—if fluid viscosities are nearly identical turbulence in the submerged jet leads to intensive mixing. Conversely, when the R_ν exceeds 400, any noticeable macroscopic entrainment does not take place. Herein we report on the modeling of free thermoviscous two-fluid shear flow with different viscosity ratios R_ν resulting from step-function temperature distribution utilizing weakly-compressible CABARET numerical method. Basing on the simulation results we analyze flow evolution in terms of the instability growth rate $\gamma = \gamma(R_\nu, \mathrm{Re})$ patterns and fields of vorticity and temperature. This work was supported by the Russian Foundation for Basic Research, grant No. 15-08-00457.

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Experimental investigation of shock wave generated instabilities in boundary layer separation region

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Boundary layer separation usually arises in the surfaces of supersonic airplanes. Separation causes pressure and thermal perturbation which can lead to control issues and surface damage.Separation

region is unsteady [1]. Thermal wall conditions influence on the separation region motion was investigated. Separation region was formed on the 23 and 30° heated ramp. Thermal boundary condition varies from adiabatic to heated wal with temperature ratio of $T_w/T_\infty = 3.11$. Velocity profiels in reattachment regions were obtained by means of Partical Image Velocimetry method. It was found that in reattachment region boundary layer is strongly preturbed and contains large scale vorticies. Reattached boundary layer is almost two times thicker than incomming boundary layer. RMS velocity fields shows velocity deviation near the separation and reattachment positions. Increasing temperature ratio causes prolongation of velocity deviation regions. Experiments have shown that heated wall condition increases instabilities in both incomming and reattachment boundary layer.

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Investigation of the influence of wave impact on methane–n-pentane mixture filtration

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The interest in the problem of the filtration of two-phase fluids modeling gas-condensate mixtures is caused by necessity to intensify the extraction of gas-condensate—valuable hydrocarbon feedstock consisting of methane and its higher derivatives. There are various flow regimes including oscillation one during the operation of the gas-condensate field [1]. It is shown that wave impact on the mixture consisting of light hydrocarbons can lead to increasing of integral flowrate of the mixture under isothermal conditions [2]. The results of experimental studies of methane–n-pentane mixture filtration in the porous medium under isothermal conditions in the

pressure range typical for the natural thermobaric conditions of gas-condensate reservoirs are shown. The effect of the periodic pressure oscillations at the output of the experimental section on the integral flowrate of the methane–n-pentane mixture is discussed. This study has done within the program of fundamental research DPEMEMCP RAS "Development of scientific principles of vibration and wave machine creation for realization of breakthrough technologies of domestic mechanical engineering" (program code IV.4.14).

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The one-dimensional problem of propagation of non-stationary waves in the theory of non-equilibrium filtration

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There are theoretical and experimental results showing the existence possibility of the periodic solutions of the gas-condensate mixture filtration problem in porous media [1, 2, 2]. In this paper consideration is given to the one-dimensional problem of the propagation of non-stationary waves in a porous medium with applying of boundary perturbances. This makes it possible to adequately calculate the quantitative parameters of the gas-condensate mixture flow process in the formation taking into account phase transition in the system. Boundary perturbance are given in the form of the Dirac delta function with the speed finiteness of non-equilibrium phase transitions and phase pressure fields coherence. A new approach

explaining the formation of periodic solutions is proposed in this paper. It is shown that such behavior is typical for gas-condensate mixtures with a retrograde region at the phase diagram and zero values of phase permeability for determinate condensate saturation. Obtained results describe filtration unsteadiness of gas-condensate fluid in real reservoirs which has been observed during their operation. This work was supported by the Russian Science Foundation (project No. 14-50-00124).

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Mathematical modeling of the various modes of two-phase filtration of hydrocarbon mixtures

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Because of reducing extraction of a dry gas deposits an active development of gas condensate fields will definitely become. Theoretical and experimental results, demonstrating the existence in filtering task periodic solution, are known. Considering gas condensate mixture as an oscillating system make possible the usage of special methods to define its main characteristics such as natural frequencies. There are many conditions of hydrocarbon production, but all of them have one common physical phenomenon—the formation of "condensate cork". Math and lab modeling can describe such process. The article contains the system of differential equations for two-phase two component mixture. The solution of it includes pressure, saturation and mass fractions. Program FlexPDE provides the system with solution, using finite element technique. As a result comparative distribution of velocity, pressure, saturation

and phase composition are received. Moreover program is able to differ equilibrium and nonequilibrium processes. Calculations show that deviation from thermodynamic equilibrium contributes gas flow rate growth and liquid flow rate reduction. Modeling in such way suppose to distinguish main physical processes, which filtering mixture depends on; give it a quantitative assessment and finally create methods leading to more effective ways of field development.

Application of fractional calculus for local non-isothermal filtration

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The mathematical description of heat and mass transfer phenomena in multiphase porous structures is complicated by the presence of non-local memory effects, strong spatial correlations and self-organization. Modeling of these processes is faced with the need to consider the non-local properties by time (memory effect) and by space (correlations effect), which is also a complicated problem. Fractional calculus opens a new direction in the theory of non-local differential equations and the possibility of fundamentally different interpretation of experimental data [2, 3].

The description of the non-isothermal filtration processes on the base of differential equations of fractional order provides the natural account for the space and time non-locality [3]. Our solution allows us to consider a number of interesting problems arising from the sharp increase in temperature and pressure up to an appearance of extreme states. Using different values of the fractional order derivatives leads to a set of solutions from which we can choose the solution that closely matches the actual filtration process.

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Seismic-acoustic noise of the Earth: Advanced understanding and research methods

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Investigation of the Earth crust deep structure, deep geodynamic processes, nonlinear interaction of physical fields, is one of the most actual problems in the World due to the fact that all the planet's geophysical processes (earthquakes, tsunami, volcanic eruptions) are activated and became an increasing threat to the citizens living in traditionally populated areas and around potentially dangerous industrial facilities. Investigation of seismic-acoustic noise by the Earth and manifestations of the telluric and planetary processes related to the movement of the Sun, Earth and Moon in the high frequency microseism structure allows to develop new approaches to solve geophysical monitoring and seismic event forecasting problems. The present world-class investigations in seismoacoustics are limited by the top frequency of the sensors (velocimeters up to 110 Hz and accelerometers up to 500 Hz), that does not allow to detect high frequency natural geoacoustic noise. The authors use the original magnetoelastic sensor to measure velocity of displacement acceleration having low self-noise level, that allows to realize a wide band of frequencies, from unities up to several thousand Hertz. High frequency microseisms structure changes due to Earth tides (solar and

lunar components), as well as under winter and summer solstices, the days of the vernal and autumnal equinox were detected. The authors obtained new data on nonlinear interactions of physical fields, deep geodynamic processes, telluric and planetary rhythms in seismic processes that allow to develop actual methods for geophysical monitoring (seismic hazard forecasting). The authors express acknowledgment to Russian Foundation for Basic Research for support of the present research by grants No. 16-05-00276 and 13-05-00041.

Model of soil cloud dynamics at impact of the asteroid Apophis to the lunar surface

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The problem aiming qualitative change of an Apophis orbit when its movements in Solar system comes to the end is formulated in [1]. Instead of passive saving tactics the variant of use of this asteroid is considered for realization of large-scale space experiment. This experiment is shock interaction of this asteroid and the Moon. Calculation of development of the soil cloud which is formed as a result of impact in the field of the Moon gravity is difficult on the basis of gas-dynamic model till times which are of practical interest. So the data obtained in a near impact zone by numerical methods of gas dynamics are used as initial data for the offered approximate model, in which the cloud is represented consisting of two independent subsystems: gas and condensed medium. Scattering is considered as axisymmetric. Particles of the medium are presented in the form of non-interacting ringlets of the known initial density and mass. The mass center of ringlet section is considered moving like a material point in the field of acceleration of the Moon gravity. Expansion of a ringlet along the radius of cross section is considered analytically.

Results of calculations of parameters of a soil cloud at perpendicular impact of Apophis to the Moon surface are given for speed 5 km/s. It is obtained that the external contour of a cloud rises up to the heights of 500 km at time 550 s, and soil cloud density changes with height from 1 g/cm^3 to practical zero.

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To the formation mechanism of the lunar mascons by galactic comets

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As a result of the famous orbital mission GRAIL, it turned out [1] that mascons can not be explained by the falling of large cosmic bodies, which have the same diameters distribution as the bodies of modern asteroid belt. This is the most important principal result, which has not yet been explained.

In the work, we present evidence that mascons are not formed by falls of single asteroids, but are created in result of bombardments by high-speed ($\sim$ 450 km/s) galactic comets. These comets have exponential size distribution and their falls have the character of "cometary showers" duration of $\sim$ 2–5 million years, repeating over 20–37 million years [2]. During of one cometary shower about of 10^4–10^6 comets can fall on the lunar surface. The flux density of galactic comets and their energy is so great that they lead to the formation of the large asthenosphere lenses of partly molten and heated rocks in the lithosphere [3, 4].

We have noticed that the lunar mascons [1] distributed according to the same exponential law as coronae on Venus [3]. Thus the explanation of mascons origin requires attraction of the physical mechanism [2–5], which could take into attention of reaction of different terrestrial planets on the falls of galactic comets.

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3. Equations of State for Matter

About electron binding energies dependence on nuclear charge and ionization state in free ions

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The analysis of the experimental and theoretical electron binding energies in the elements of the periodic table from neon to uranium has been before carried out [1]. As a result some ordering of electron levels in the closed shells of neutral atoms has been established. The ordering enables to construct the two independent on the atomic number Z functions, which one can use to estimate electron binding energies in a free atom. In the report this approach is applied to analyze a dependence on the atomic number of electron binding energies in free positive ions. The Thomas–Fermi (TF) model and Bohr–Zommerfeld condition are used to determine the electron levels in an ion with a charge z, the ion TF function depending on an ionization state $\alpha = z/Z$. The analysis of the s-state electron levels demonstrates both the atomic number and ionization state scaling in ion closed shells. The binding energies in some free ions of the elements from neon to barium calculated by the many configuration Dirac–Fock model (MCDF) are analyzed to verify the similar regularities in the results of more expanded quantum-mechanical models.

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Electron core ionization in compressed alkali and alkali-earth metals

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Elements of groups I and II in the Periodic table have valence electrons of s-type and are usually considered as simple metals. Crystal structures of these elements at ambient pressure are close-packed and high-symmetry of bcc- and fcc-types, defined by electrostatic (Madelung) energy. Diverse structures were found under high pressure with decrease of the coordination number, packing fraction and symmetry. Formation of complex structures can be understand within the model of Fermi sphere—Brillouin zone interactions [1, 2] and supported by Hume–Rothery arguments. With the volume decrease there is a gain of band structure energy accompanying by formations many-faced Brillouin zone polyhedrons. Under compression to more than a half of the initial volume the interatomic distances become to be close or smaller than ionic radius, what should lead to the electron core ionization. At strong compression is necessary to assume for alkali and alkali-earth metals the valence electron band overlap with the upper core electrons and increase the valence electron count under compression.

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High-temperature chemistry in low-temperature environment

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Experimental study of chemical processes of refractory metals, such as W, Rh and Mo, as well as of Carbon, for obvious reasons, causes considerable difficulties. Our paradoxical approach is the study of such processes in superfluid helium (He II) at extremely low initial temperature. The paradox is that He II is the quantum fluid with extremely high thermal conductivity. So, no local overheating was considered to be possible there and all processes between particles should be strictly isothermal. This suggestion turned out to be fundamentally wrong. He II high thermal conductivity takes place only at heat fluxes less than 3 W/cm^2. In the meantime to prevent the overheating during two small metal nanoclusters coalescence the flux of at least 10^6 W/cm^2 is necessary. As a result, the liquid around the reagents evaporates forming a heat insulating jacket of low density gas. For the direct proof of such scenario the thermal emission accompanying coagulation of metal atoms in He II has been experimentally studied. It was shown that the brightness temperature in the early stages of the coagulation ever exceeds the melting point of these metals, accounting for W, Mo and Pt around 4000 K, 3500 K, and 3000 K correspondingly. Several important properties of metallic nanostructures were revealed such a way: (i) The instability of metallic nanospheres associated with the high negative pressure developed within them under rapid cooling. (ii) The low temperature stability of ultrathin nanowires due to Rayleigh instability induced by thawing the surface mobility of the atoms. (iii) Formation of core-shell- and nano-hetero-structures by coagulation of binary alloys. (iv) Formation of onion-like structures and nano-diamonds under carbon coagulation.

To the Birch law for liquid metals

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The sound speed is an important thermodynamic characteristic of matter. It defines the typical temporal scale in phenomena arizing upon extreme conditions in a substance. The Birch law is an empirical relation in the liquid state of matter. According to this law, the sound speed of liquid material can be approximated by linear function of density. We present examples of Birch law for liquid metals and discuss the region of its applicability.

A model of wide-range equations of state for matter at high energy densities

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A model of wide-range equations of state for matter at high energy densities is proposed. It has a form of functional relation between specific internal energy, pressure and density. Based on the model, equation of state, which is in a good agreement with data from shock-wave experiments over whole investigated region of pressures and internal energies, is constructed for aluminum. Comparison of calculated results for the metal with the data is presented.

Quantum-statistical calculations of shock compressibility of three metals at high pressures

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Many experimental data on shock compressibility of a wide variety of substances at ultra-high pressures were obtained by relative measurements. In contrast to absolute measurements, the shock-wave velocities were registered only as the wave passed successively through layers of the investigated substances. The determination of the wave parameters in one of the layers is based on a solution of the problem of the discontinuity decay at the contact [1], and requires knowledge of the equation of state of the other layer. The interpretation of these experiments was based on Hugoniots for standard materials (Al and Fe) calculated by using a model equation of state.

In the present work, different quantum-statistical models [2] were used to obtain shock adiabats for standard materials. Investigation of influence of choosing theoretical model at ultra-high pressures, where shell effects have most strongly effect, was carried out. On the basis of the current calculations in comparison with measurement results, specified data of shock compressibility of Al, Fe and Cu were obtained.

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Applications for the equation of state based on the Thomas–Fermi model with corrections

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Physics of extreme states of matter usually deal with phenomena which cover wide region on a phase diagram. To describe them properly the consistent equations of state for matter are required. At high temperatures about tens of eV one have to account large number of electron states using most precise density functional theory (DFT) based approach what can be computationally expensive. From the other hand, the quite simple Thomas–Fermi approach with quantum, exchange [1, 2] and shell corrections [3] was found to be realistic enough in such conditions [4]. Though the calculation of shell corrections requires evaluation of semiclassical electron energy levels, the developed approach [5] with boundary energy between discrete and continuous spectrum is applied to restrict number of states and keep consistent thermodynamics. We demonstrate agreement between the Thomas–Fermi model and DFT calculations of electron pressure at normal density isochore. The advantage of using shell corrections is equations of state also corresponds well Saha model data for low density plasma. Additional applications for the Thomas–Fermi method are discussed.

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Temperature anomalies of shock waves and adiabatic flows in hot nuclear matter

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The temperature anomalies of shock and adiabatic compression and rarefaction in the presence of quark–hadron phase transition are considered. Within the framework of the widely used phenomenological approach to construct the equation of state of hot nuclear matter, which combines statistical description of the hadron gas and the MIT-bag equation of state of quark–gluon plasma, the procedure of its thermodynamic properties calculation has been realized. The features of this approach, related to the application of the excluded volume method in its thermodynamically consistent form [1], are analyzed. The shape of the Taub adiabat [2] and isentropes in the phase diagram is characterized by the pressure decrease with temperature along the curve of phase equilibrium. The segments of the adiabats that belong to the two-phase region have negative slope in the temperature-density plane. This behavior leads to the following anomaly of the adiabatic and shock-wave processes. The high pressure phase (the quark–gluon plasma) has lower temperature than the low-pressure one (the hadronic matter) in the composite compression and rarefaction waves. The one-dimensional problems of adiabatic expansion layer of quark–gluon plasma and compression of hadronic matter is solved. The details of the anomalous wave dynamics associated with the occurrence of the composite compression and expansion waves, as well as features of the temperature behavior in this processes, are described.

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Specific electrical conductivity of sapphire at shock compression up to 600 GPa

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Monocrystalline sapphire is widely used as insulator in experiments on measurements of the electrical conductivity of single and multiple-shock compressed matter. However, direct measurements of electrical resistance of shock-compressed sapphire were performed only up to 220 GPa [1], where it was shown that already at 300 GPa asymptote will reach 10000 S/cm and sapphire lose insulating properties. In this talk the new data on electrical conductivity of monocrystalline m-cut sapphire under shock compression up to 600 GPa will be presented. The conical cumulative generators of shock wave, analogous to [2], but with increased explosive mass and enhanced parameters, were used for shock loading of measuring cell. 3-electrodes scheme of resistance measurements was used. Optical multi-channel pyrometry and fast optical detectors were used to measure shock velocity and brightness temperatures in sapphire sample. The data obtained shows, that even at 600 GPa electrical conductivity of sapphire do not exceeds 20 S/cm, that opens possibility to use it as an insulator for measurement of electrical properties of compressed hydrogen.

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Combined laser ultrasonics, laser heating and Raman scattering in diamond anvil cell system

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There is widespread interest in the elastic properties of solids at elevated temperatures and high pressures. Laser ultrasonics (LU) combined with diamond anvil cell (DAC) demonstrated to be an appropriate technique for direct determination of the acoustical properties of solids under high pressure. The use of lasers generating nanosecond acoustical pulses in solids allows measurements of the velocities of shear and longitudinal waves in iron up to 23 GPa. In this report, we describe development of a multi-functional *in-situ* measurement system under high pressure equipped with a laser ultrasonics (LU) system, Raman device, and laser heating system (LU-LH) in a diamond anvil cell (DAC). The system is unique and allows us to: (i) measure shear and longitudinal velocities of non-transparent materials under high pressure and high temperature (HPHT); (ii) measure temperature in a DAC under HPHT conditions using Planck's law; (iii) measure pressure in a DAC using a Raman signal; and (iv) measure acoustical properties of small flat specimens removed from the DAC after HPHT treatment. We demonstrate that the LU-LH-DAC system allows measurements of velocities of the skimming waves in iron at 2580 K and 22 GPa.

In-situ measurement of the high temperature distribution inside diamond-anvil cell by acousto-optical spectral imaging system

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The laser-heated diamond-anvil cell (LH-DAC) is the only experimental tool able to create extreme static pressures ($P > 100$ GPa) and temperatures ($T > 3000$ K) and therefore it is widely used in high-pressure research and geophysics. Further progress in the development of the laser heating techniques requires the knowledge of the two-dimensional (2-D) temperature field in a material induced by laser beam radiation. Recently it was shown that imaging tandem acousto-optical tunable filter (TAOTF) synchronized with a video camera allows *in-situ* measurement the 2-D temperature distribution over the surface of microscopic specimens [1]. The objective of this research is to demonstrate that TAOTF spectroscopic system can be used for the measurement of the real 2-D temperature distribution in LH-DAC. The 2-D temperature distribution $T(x, y)$ of the heated g-C_3N_4 was obtained from ten spectroscopic images taken at different wavelengths by fitting the actual signal to Planck's equation at each point of the specimen's surface. In this study, we assume the variation of the specimen's emissivity to be small over the spectral tuning range and the measured temperature range.

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Combined laser heating and Raman scattering in diamond-anvil-cell system

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In the present report, we describe development of a multi-functional *in-situ* measurement system under high pressure equipped with a Raman device, and laser heating system (LU-LH) in a diamond-anvil cell (DAC) in the Scientific and Technological Center of Unique Instrumentation of the Russian Academy of Sciences. The system consists of three components: (1) fiber laser, which is designed to allow precise control of the total power in the range from 2 to 100 W by changing the diode current, for heating samples; (2) spectrometer for measuring the temperature of the sample (using black body radiation), fluorescence spectrum (spectrum of the ruby for pressure measurement), and Raman scattering measurements inside a DAC under high pressure and high temperature (HPHT) conditions; and (3) optical system to focus laser beams on the sample and image it in the DAC. The system is unique and allows us to: (i) heat specimen by a laser in a DAC and to measure temperature in a DAC under HPHT conditions using Planck's law; (ii) measure pressure in a DAC using a Raman signal; and (iii) measure Raman scattering of specimen under high pressure and of small flat specimens removed from the DAC after HPHT treatment.

Structure of amorphous carbon quenching from liquid in the pressure range 1–40 GPa

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It is well known that quenching from the liquid state is the basis of many methods for creating new materials with unique properties. Polymorphism of liquid and amorphous carbon results in the fact that they represent a mixture of atoms with different states of hybridization: sp^1, sp^2, sp^3. According to the literature there is a tendency of growth of sp^1-atoms in liquid and amorphous carbon with decreasing pressure. Great interest to the carbine and pseudocarbynes, consisting of sp^1-hybridizing atoms sharply increased recently. These materials have unique optical and mechanical properties. In the present work the pressure dependence of the structure of amorphous carbon, quenching from liquid in the range of 1–40 GPa, studied by molecular dynamics simulation using software package LAMMPS. The initial simulation cell was a cube with an edge of 42.9 Åwith periodic boundary conditions. The interaction between the carbon atoms was determined by two bond-order potentials: Airebo and ReaxFF. Such potentials take into account the order of the chemical bonds, the breaking and formation of new chemical bonds during the modeling process. To investigate the influence of pressure on the structure of amorphous carbon we study the bulk quenching from liquid carbon in the NPT ensemble at constant pressure. First of all, we are interested in how the distribution of chemical bonds, sp^1–sp^2–sp^3 in amorphous carbon depends on pressure during the quenching. This work was supported by the Russian Foundation for Basic Research (grant 16-08-01295).

Highly oriented pyrolytic and natural graphite under high pressure

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Studies of baric dependence of resistivity of highly oriented pyrolytic graphite (HOPG) and natural graphite were carried out at room temperature. The pressure was applied by means of a diamond-anvil cell with electrically conductive anvils of the "rounded cone-plane" type made of synthetic polycrystalline diamonds "carbonado". The resistance measurements were carried out in a course of loading–unloading cycles in the pressure range from 15 GPa to 50 GPa. The resistances of HOPG samples were also measured in the pressure range from 5 GPa to 27 GPa. Characteristic times of resistance relaxation were determined to be from 20 minutes to several hours. Characteristic features of both HOPG and natural graphite are the decrease of resistance by more than 2 times and hysteresis in pressure the dependence of resistance. All features became more pronounced for thinner samples and lower current.
This work was supported by the Russian Foundation for Basic Research (grant 16-02-01137).

Amorphization of the fullerenes C_{70} at high pressures

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We report the results of experimental studies crystals of the fullerene C_{70} at pressure up to 50 GPa and room temperature. *In-situ* high pressure Raman spectroscopy and x-ray diffraction showed changing in the crystal structure of the fullerene C_{70} at pressures above

14 GPa. Electrical properties of C_{70} were studied at pressure up to 50 GPa. The results Raman spectroscopy and electrical measurements indicates that the amorphization of fullerenes is reversible in pressure range below of 30 GPa. Pressure dependences of crystals C_{70} resistance obtained at pressures up to 48 GPa indicate the irreversibility of structural transformations taking place in the sample at a pressure of $\sim$ 50 GPa.
This work was supported by the Russian Foundation for Basic Research (projects 16-02-00857 and 16-02-01137). The authors are very grateful to Prof. L.S. Dubrovinsky (University Bayreuth, Germany) for the possibility to carry out of high pressure Raman measurements.

Investigation of magnetoresistance of polycrystalline In- and Cu-chalcogenides at the high pressure up to 50 GPa

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This work is devoted to the study of behaviour of electroresistance R_e and magnetoresistance R_m of semiconductor polycrystalline materials: $CuInAsS_3$, $CuInAsSe_3$, $CuInS_2$ and $CuInSe_2$ under high pressures up to 50 GPa in a constant transverse magnetic field. The high pressures up to 50 GPa were produced in the high-pressure cell (HPC) with the anvils of carbonado-type artificial diamonds with good conductivity that make it possible to examine the electrical properties of samples placed into HPC. The constant transverse magnetic field was produced by a testaceous electromagnet, the value of magnetic induction varied from 0 to 1 T.
Baric intervals in which there are significant changes in the behavior of electric and magnetoresistance were established. The decrease electrical resistance is observed with pressure increasing for all studied materials. Pressure ranges in which the $R_m < 0$ were found.

Baric intervals in which there are extrema on the dependencies of $R_e(P)$ and $R_m(P)$ that may be associated with the structural changes in studied materials were determined. These data are in agreement with previously studies of others electro-physical parameters of these compounds [1–3].
The study was supported by the Russian Foundation for Basic Research (projects 16-02-00857 and 16-02-01137).

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High pressure influence on electrical properties of multicomponent polycrystalline materials based on copper and germanium selenides

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This work is devoted to the high pressure P up to 50 GPa influence on the electroresistance R and magnetoresistance R_m of the polycrystalline material $(GeSe)_x(CuAsSe_2)_{1-x}$, $x = 0.5$ ($CuGeAsSe_3$). The materials $(GeSe)_x(CuAsSe_2)_{1-x}$ are well known semiconductors with interesting thermal and baric dependences of electric properties [1, 2].
The pressure dependences of the investigated material electric properties were studied in a transverse magnetic field up to 1 T. High pressures have been achieved using the high pressure cell described in detail in paper [3].
It was found that the electroresistance of $CuGeAsSe_3$ decreases on 2 orders with pressure increasing from 16 to 42 GPa. The phenomenon of negative magnetoresistance (up to ∼25% in modulus) is observed for this material. Several extremes on curve $R_m(P)$ are observed for the material $CuGeAsSe_3$ as well as for materials $(GeS)_x(CuAsS_2)_{1-x}$

[4], and R_m extremes pressures correspond to the baric intervals of the other electrical properties behavior features.
The study was supported by the Russian Foundation for Basic Research (project No. 16-02-00857).

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The temperature and high-pressure effects on the dielectric properties of materials based on perovskite-like oxides

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The work is devoted to investigation of dielectric properties of new synthesized ceramic materials $La_{2-x}Sr_xNi_{1-y}M_yO_4$ (M = Co, Cu, Fe) in terms of fixed and variable electric fields to determine the effect on the electrical properties of external influences: the synthesis conditions (thermobaric treatment), concentration, frequency of electric field, temperature, pressure [1, 2]. The real part of the dielectric constant of $La_{2-x}Sr_xNi_{1-y}M_yO_4$ (unexposed thermobaric treatment) remains constant $\sim 10^2$ and varies only slightly with frequency in the region of 10^3–10^7 Hz, while the same materials subjected thermobaric treatment have the dielectric constant $\sim 10^3$. The materials are characterized by activation-type conductivity in the investigated temperatures. The activation energy is 0.10–0.12 eV. High-pressure effect on electrical properties revealed irreversible, and resistivity values of the direct process do not match with the values of reverse process. It suggests the change in the crystal structure with increasing pressure is also irreversible. The impact

of high pressure on the crystal structure and physical properties for oxides with perovskite-like structure of K_2NiF_4-type requires further research [3]. Research is supported by the Russian Foundation for Basic Research (grants 16-02-00857 and 17-03-00150).

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Effect of high pressure on dielectric properties of the material with high dielectric constant $CaCu_3Ti_4O_{12}$

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Currently scientists have been offering a lot of models what explain reasons of high dielectric constant (10^4–10^5) in $CaCu_3Ti_4O_{12}$ (CCTO). This models are used for explanation high dielectric constant of materials which are not ferroelectrics [1–3]. But currently the unified theory of explaining dielectric constant has not been developed. Now we are presenting results of research effect of high pressure on dielectric properties of the material with high dielectric constant CCTO which was synthesized in conditions of high pressure and high temperature ($P = 80$ kbar, $T = 1100$ °C, $t = 14$ min). X-ray studies displayed that material crystallizes in cubic symmetry and has perovskite-like structure. Dielectric properties of CCTO were researched at pressure from 3 to 27 GPa. With increasing pressure the tangent of dielectric loss and the conductivity changed exponentially and increased about 2-fold. The conductivity relaxation time decreased about 6-fold. The dielectric constant remains high. Results confirm that internal effects (processes of space-charge polarization) related with structural distortions of polyhedral [1, 4] have a significant influence on the formation of high values dielectric

constant. This work was supported partly by the Russian Foundation for Basic Research (grants No. 16-02-00857 and 15-03-00868).

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Influence of high pressure on the electrical properties of perovskite-like vanadium-containing oxide

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$CaCu_3Ti_4O_{12}$ (CCTO) is a dielectric material that was intensively studied in the past decade because of its large effective dielectric permittivity and the low-temperature dependence of permittivity [1]. The purpose of this paper is to study the electrical properties of perovskite-like structures such as $CaCu_3Ti_{4-x}V_xO_{12}$ (x = 0.1–0.5 and x = 4) in the pressure range of 10 to 50 GPa at room temperature. CCTO has been discussed as an alternative dielectric for multilayer ceramic capacitor applications. CCTO and $CaCu_3V_4O_{12}$ (CCVO) are double perovskites and crystallize in cubic space group "Im-3", Z = 2 parameters of a = 7.396 Å and a = 7.284 Å respectively. When doping titanium vanadium observed decrease in the average grain size, the decrease of the lattice parameter, the crystalline syngony is not changed. One of the main properties CCVO and CCTO is that with increasing pressure P, the electric resistance (R) monotonically decreases in the subsequent decrease pressure, R is returned to the previous values. CCTO characterized the semiconductor conductivity, but CCVO—metallic conductivity. Notwithstanding different conductivity types and electronic structures, the dependence $R(P)$ for CCTO and CCVO qualitatively the

same. This work was supported partly by the Russian Foundation for Basic Research (grants No. 16-02-00857 and 15-03-00868).

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Hydrogen solubility in amorphous silicate $Mg_{0.6}SiO_{2.6}$ at pressures up to 75 kbar

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The mantle is mostly composed of silicates of such elements as Mg, Fe, K, Al and Na. Pressure-induced phase transformations in silicates therefore play a key role in the processes occurring in the Earth interior. Our understanding of these processes will be incomplete in the absence of physical and chemical data about the interaction of silicates with hydrogen at high pressures, because the Earth crust and upper mantle contain a lot of light elements including hydrogen. The solubility of molecular hydrogen in silicate glass $Mg_{0.6}SiO_{2.6}$ has for the first time been investigated at high hydrogen pressures by thermobaric quenching. The molar ratio H_2/f.u. is found to nonlinearly increase with pressure from $X = 0.12$ at $P = 10$ kbar to $X = 0.303$ at $P = 75$ kbar and $T = 250°$C. An investigation of the quenched samples by Raman spectroscopy shows that hydrogen in the amorphous $Mg_{0.6}SiO_{2.6}$ is dissolved in the form of H_2 molecules that manifests itself by a bands of stretching H-H vibrations at near 4163 and 4173 cm^{-1} in the spectra of the samples synthesized at $P = 47$, 56, 61 and $P = 66$ kbar. The bands at 345 and 590 cm^{-1} are close to the rotational lines S(0) at 353 cm^{-1} and S(1) at 586 cm^{-1} of free H_2 molecules. Also, the results of the Raman spectroscopy and x-ray diffraction studies suggest that in the pressure interval 52.5–61 kbar, the $Mg_{0.6}SiO_{2.6}$–H samples experience a phase transition to a denser amorphous modification.

Despite the increased density of the amorphous $Mg_{0.6}SiO_{2.6}$, its hydrogen content continued to grow at hydrogen pressures above 61 kbar.

Preparation and investigations of nanocluster compounds with hydrogen bonds

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The work is devoted to the phase transitions studies of nanocluster compounds with hydrogen bonds on the example of ethanol and ice. Nanocluster compounds are obtained by vapor-deposition on the superfluid He-II surface. The studies are performed using of X-ray, neutron and calorimetric methods which demonstrate the amorphous states of prepared materials. Amorphous samples containe nanocluster particles with a characteristic size 6–10 nm as according to neutron scattering analysis. It is found that the transformation of the nanocluster into the powder state occurred at a temperature $T \approx 90$–100 K (for deuterium alcohol). The detail structural analysis demonstrate that the nanocluster ice samples are multi-phases. There are three phases in the initial sample: amorphous ice, cubic ice and hexagonal ice. Calorimetric measurement shows three phase transitions in these samples during heating in a temperature range from 120 K to 250 K. The first and second transitions occur in temperature range of 140–150 K. However, calorimetric peaks of these transitions are strongly overlapped which do not allow us correctly calculate thermal effects for each transition. Third calorimetric peak in the range from 180 K to 200 K can be attributed to the transition from cubic to hexagonal ice. Neutron research are necessary to study the structural features of the initial amorphous state and crystalline phases formed during heating of the nanoclusters.

Influence of the hydrogen bonding degree on the elastic properties of propylene glycol oligomers under high pressure

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Hydrogen bonds play an important role in the intermolecular interaction of molecular glassformers [1]. Molecules of the investigated substances (mono-, di- and tripropylene glycol) have different weights and lengths, but the number of the hydroxyl OH groups remains constant and equals to 2 [2]. We have studied the elastic properties of the oligomers of propylene glycol under high pressure in liquid and glassy state, and at the glass–liquid transition in order to determine the effect of the specific amount of hydrogen bonding on the elastic properties. Propylene glycol oligomers were studied under high pressure up to 1 GPa in liquid state (at room temperature) and up to 1.8 GPa in glass ($T = 77$ K). All three investigated substances have similar compressibility both in liquid and glassy state. Di- and tripropylene glycol have close values of the shear modulus G and the bulk modulus B, but both are considerably lower than the elastic moduli of monopropylene glycol. Isobaric warming from 77 K to room temperature revealed a monotonic dependence of the elastic moduli and glass transition temperature Tg from the mass of the molecules. We can conclude that a high intermolecular cooperativity, due to the large specific number of hydrogen bonds (like in propylene glycol), leads to strengthening of elastic moduli.

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Polymorhous and phase transitions in high-purity Mg-95 according to sound velocity measurements

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Sound velocities in the shock-compressed high-purity Mg-95 as of GOST 804-93 were measured within 20–70 GPa and these measurement results are reported. Optical analyzer technique [1–3] was used to record processes in the catch-up release experiments. In the above-mentioned range, the material melting is shown to proceed at the shock front. Melting is estimated to start at 50 GPa and to terminate at $\sim$ 55 GPa. The hcp–bcc transition is assumed taking place within 20–30 GPa, which agrees with numerically simulated estimations [4].

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Quantum calculation of thermodynamic and transport properties of CH_2 plasma

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This work covers calculation of radial distribution functions, specific energy and static electrical conductivity of CH_2 plasma in the two-temperature regime. The calculation is based on the quantum molecular dynamics, density functional theory and the Kubo–Greenwood formula. The properties are computed at 5 kK $\leq T_i \leq T_e \leq$ 40 kK and $\rho = 0.954$ g/cm^3 and depend severely on the presence of chemical bonds in the system. Chemical compounds exist at the lowest temperature $T_i = T_e = 5$ kK considered; they are destroyed rapidly at the growth of T_i and slower at the increase of T_e. A significant number of bonds are present in the system at 5 kK $\leq T_i \leq T_e \leq$ 10 kK. The destruction of bonds correlates with the growth of specific energy and static electrical conductivity under these conditions.
The main results of this work were published in paper [1].

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Calculation of entropy in classical and first-principles molecular dynamics simulation

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The first-principles calculation of entropies and free energies for liquids and the determination of liquid–solid phase boundaries is a long-standing problem in molecular dynamics and one that has received considerable attention with a variety of approaches.
We present a detailed analysis of entropy reconstruction from a velocity autocorrelation function in molecular dynamics simulation for solid and liquid states. The reconstruction is based on the vibrational density of states (VDOS) and for the liquid phase is known as a two-phase thermodynamic (2PT) model. We compare this method with more complicated technique of thermodynamic integration. We also present results of *ab initio* calculations of melting curve and isentropes using 2PT model for various metals.

Reconstruction of release isentropes based on first-principles simulations

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One of the most important problems in modern physics is the study of thermodynamic properties of materials under extreme states.

This is necessary both for the construction of wide-range equations of state of materials at high temperatures and pressures, and for solving of a lot of applied and fundamental tasks. The development of computational methods and supercomputers made it possible to obtain reliable data about thermodynamic properties of substances as a result of an *ab initio* approach—the method of quantum molecular dynamics (QMD).
The goal of this work is to study methods of reconstruction of isentropic expansion curves based on QMD simulation data. We analyze accuracy and computational complexity of three methods: Zel'dovich approach [1], method of re-shock Hugoniots and direct calculation of entropy using a two-phase thermodynamic (2PT) model [2]. In the first method, an ordinary differential equation for the temperature is solved numerically. The second method is based on the feature of the second-order contact of a re-shock Hugoniot and release isentrope. The density of vibrational states which is reconstructed from a velocity autocorrelation function is used to calculate entropy in the third method.
In this work aluminum and molybdenum were used as examples. Calculated release isentropes by three methods are close to each other and agree well with experimental data.

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Investigation of structural and thermodynamic properties of Ni–Al

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High-density reactive materials (HDRM) are increasingly used in different areas of science and technology. These materials undergo a self-sustained exothermic reaction upon initiation through a shock

or thermal loading and do not need additional reagents, that allows to use HDRM as a fuel, welding, combustion and detonation initiator. Ni–Al systems are an important subclass of HDRM, because the product of the reaction is an intermetallic compound with high resistance to temperature and oxidation.
In this work, structural and thermodynamic properties of the solid and liquid Ni–Al compound are studied using the ab initio method of quantum molecular dynamics (QMD). The simulations were carried out for 700–3000 K temperature range and atmospheric pressure. Pair correlation functions are analyzed to determine the presence of chemical bonds Ni–Al. Diffusion coefficients for individual components are also calculated.
Another goal of this work is the investigation of the reaction propagation in thermally-initiated Ni–Al foils. For this purpose, we performed QMD simulations of Ni–Al layers in the microcanonical (NVE) ensemble. An exothermic reaction between solid Ni–Al layers is observed in our simulations at temperature less than the melting temperatures of the components.

Evaluation thermodynamic properties of metals by the perturbation theory

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The development of theoretically equations of state (EOS) of substances based on the modern methods of statistical mechanics and realistic interaction intermolecular potentials provide good agreement with the results of Monte Carlo simulation (MC) and molecular dynamics (MD). An example of the successful application of perturbation theory KLRR [1] are developed in [2, 3] EOS of fluid systems, which provides the good agreement results of calculations thermodynamic properties of fluid and parameters of shock-wave compression with the simulation data (MC and MD) and the experimental data at high pressure and temperatures [4,5]. In this report

we first demonstrated the use of the EOS [2] to calculate the properties of aluminum in an isothermal compression. For a description of the interatomic interaction in metals used Morse pair potential. The calculation results are in good agreement with the experimental data and calculations based on empirical equation of state described in the literature. Thus, EOS based on the perturbation theory with a suitable interatomic potential is a reliable universal tool for the calculation of the thermodynamic properties of a gas (fluid) systems and condensed matter and allows to analyze the dynamics of changes in the atomic structure and phase transformations of matter during heating and compression. This work is supported by the Russian Science Foundation (grant 16-19-00188).

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

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The "jellium" approximation i.e. replacing system of discrete particles (electrons and ions) by hypothetical "fluid" with pure local

properties (i.e. depending on local density only) is widely used not only in hydrodynamic applications but also in thermoelectrostatics i.e. in calculation of equilibrium charged particles distribution near a source of non-uniformity. The local in local equation of state (EOS), that connects local pressure, energy and chemical potential of charged particles with local density and temperature, is used for this purpose. In most cases it is ideal-gas (correlationless) EOS approximations (i.e. Thomas–Fermi or Poisson–Boltzmann approximations). The main problems of this approach is correct taking into account of mean-particle correlations (non-ideality). We provide calculations and discuss the results for charged particle equilibrium distribution in case when we use non-ideal EOS for one-component electronic or ionic systems. The main result of such using of non-ideal EOS is appearance of discontinuities in equilibrium spatial profiles of non-uniform charge distribution. Features and parameters of these discontinuities are discussed and illustrated. This work was supported by the Russian Scientific Foundation (grant 14-50-00124).

Anomalous charge profiles in thermoelectrostatics and phase transitions in Coulomb models

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The main problem of thermoelectrostatics, which consists in calculation of equilibrium spatial charge profile in non-uniform Coulomb systems, is under discussion. It is, for example, equilibrium electronic profile in average atomic cell, spatial profile of microions in special trap or microions profile around central macroion in Wigner–Seitz cell etc. General way for solution is variational approach of statistical mechanics (non-reduced version of density functional theory). The main problem on this way is correct taking into ac-

count inter-particle correlations (non-ideality). We discuss anomalies, which appear in all the charge profiles when one uses *local* equations of state (EOS) approach (quasi-uniformity approximation) i.e. local EOS, corresponding to the exact non-ideal macroscopic system of Coulomb particles (one-component plasma model—OCP). For instance, it is electronic fluid (jellium) in Thomas–Fermi approximation or ionic fluid in one-component charged hard spheres model etc. The main statement of this work is that we should use for this purpose the local EOS for *modified* OCP models of nonideal electronic (or ionic) fluid on *uniformly compressible* electrostatic compensating background—OCP($\sim$). The basic problem in this case is presence of three phase transitions in the model OCP($\sim$). It is claimed that these phase transitions in EOS of OCP($\sim$), as macroscopic non-regularities, manifest itself at micro-level as *discontinuities* in equilibrium spatial profiles of non-uniform charge distribution. Features and parameters of discontinuities are discussed and illustrated for real examples of thermoelectrostatic problems. Supported by the Russian Science Foundation (grant No. 14-50-00124).

Revealing free-like electrons in density functional theory models of warm dense matter

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Quantum mechanical description of electrons in condensed phase is a general problem of the highest importance. However the rigorous wave-functions based theory is very complicated even for ground state ($T_e = 0$), the finite temperature (FT) case being much farther from applicability in practice. Only recently accurate quantum Monte Carlo approaches have been developed in this field [1]. That

is why the Kohn–Sham density functional theory (KS DFT) method in the FT formulation became a tool of choice. Temperature implies the necessity of the statistical description of the coupled system of electrons and ions using the free energy F as a starting point for the theory. At the atomistic level one needs to describe the ion dynamics and therefore to know how to calculate forces acting on them. Previously [2, 3] we have presented the results those raised questions about how we should bridge the FT KS DFT description with classical atomistic scale. In this talk we review the free energy models that are deployed in ab initio theory of WDM in equilibrium and non-equilibrium cases and provide our novel results on the analysis of the interatomic forces and pressure in WDM.
The study has been supported by the Russian Academic Excellence Project "5-100".

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Features of phonon density of states and dispersion curves in uranium

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Velocity of defect motion in solid states is connected with vibration properties of the lattice. Thus, it is useful to know phonon density of states (PDOS) and dispersion curves for computation of defect diffusion [1]. Phonon density of states can be calculated from the dynamical matrix [2] of the system or from the velocity autocorrelation function [3]. One can also build the dynamical matrix in the reciprocal space directly from the molecular dynamics simulations using Green's functions. This way allows to find phonon density of states in particular directions and dispersion curves [4]. In this work phonon density of states and dispersion curves were

calculated for clear lattice of alpha and gamma uranium as well as for lattice with a defect. Computations were made by molecular dynamics software LAMMPS and additional tool "phonon", EAM potential was used [5]. Aforementioned methods were compared and the limits of applicability were stated. Dependence of PDOS and dispersion curves on temperature at constant temperature were obtained. The connection between phonon spectrum softening and abnormal diffusion coefficient in the direction $\langle 111 \rangle$ for bcc lattice of gamma uranium was analyzed. The work was supported by the Russian Science Foundation (grant 14-50-00124).

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Electronic structure calculations for defects in γ-uranium

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Advances in nuclear energy applications are obviously connected with the development of new materials with unique properties. Radiation damage in structural materials and nuclear fuels is an important topic of research for the improvement of the technologies of nuclear power plants. A description of radiation damage requires knowledge of the atomistic mechanisms of defect generation in solids.
The basis of such a description at the atomic level is the electron density functional theory (DFT), which has been used successfully for

a long time. Since actinide atoms have many electrons, all-electron calculations are possible only for small molecules. Pseudopotentials are needed to successfully model condensed actinide-bearing materials. However, there is only a limited set of properly described pseudopotentials suitable for DFT calculations with actinides. Relativistic effects and strong electron correlation effects in the 5f states are important for building reliable pseudopotentials of actinides. In this work we describe the generation of a pseudopotential for a uranium atom in the format suitable for the ABINIT and CP2K codes (free alternatives to VASP). The accuracy of this pseudopotential is illustrated by a series of molecular and solid-state calculations. This pseudopotential was used to calculate energy of defects in gamma uranium. The results are compared with VASP code.
The work was supported by the Russian Science Foundation (grant No. 14-50-00124). The authors acknowledge the Joint Supercomputer Centre of RAS and the Supercomputer Centre of JIHT RAS for providing computing time.

Calculation of the vacancy diffusion rate in bcc U and Mo

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Migration of point defects determines many microscopic processes in nuclear materials: climbing of dislocations, diffusion of fission products, formation of bubbles and swelling. Experimentally measured self-diffusion is a combination of effects of vacancies and interstitials, but in bcc metals the impact of vacancies is much higher. Calculation of the vacancy diffusion rate is important for building a mesoscale model of the evolution of fuel in reactor conditions. The generally accepted model for temperature dependence of diffusion of defects is the Arrhenius equation $D = D_0 \exp[-E_a/(k_B T)]$, where E_a is a free energy barrier and D_0 is a frequency factor, determining

an effective frequency of jump attempts [1]. However, bcc metals shows wide range of diffusion rate values comparing to fcc metals, and some of them like γ-U shows also deviation from linear law in Arrhenius coordinates [2]. Researchers also discuss temperature effects on the vacancy formation volume and consecutive effects on the mobility of vacancies [3]. This work shows that the molecular dynamics simulation of the motion of defects in bcc metals reveals the deviation from the Arrhenius law. Temperature dependence of the migration energy is discussed, and the method for the accelerated calculation of this dependence is considered. The work is supported by the Russian Science Foundation (grant 14-50-00124).

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Point defects properties in atomistic models of bcc tantalum

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This work is dedicated to the study of the point defects properties in atomistic models of bcc Ta. Molecular dynamics simulations of Ta were applied by embedded atom model (EAM) and spectral neighbor analysis potential (SNAP) [1] model. All simulations were carried out in the NVE ensemble with the molecular dynamics package LAMMPS. The required parameters of the EAM and SNAP models for Ta from [1] and [2] respectively. We performed the computations of lattice constant and bulk modulus. The comparison of the calculated values with experimental data shows that the EAM and SNAP models reproduce the experimental value with a good accuracy, as well as the lattice constant. However, we found that

the SNAP model predicts the slope of the temperature dependence of the bulk modulus incorrectly. We calculated the barrier energy of point defect migration at $T = 0$ for both models by nudged elastic band method. The calculated values show that both models give the similar values. Also, we compute the barrier energy of point defect migration considering the non-zero temperature by metadynamic [3] method.

The study has been funded by the Russian Academic Excellence Project "5-100".

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Influence of the uniaxial compression on position of hydrogen atoms diffused in body-centered cubic Fe

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Hydrogen diffusion coefficient depends considerably on the stresses applied to it and has a special importance for predictions of the hydrogen degradation processes. As shown in the work [1], biaxial tension (compression) of the bcc Fe in the [100] and [010] directions by 6% (4%) with compression (tension) along the [001] direction by 19% (13%) result in the conditions at which occurs the hydrogen transition from tetrahedral (T) site to octahedral (O) site. Theoretical conceptions on the behavior of the supercell as a macro object, used in this paper work, have no grounds and may have resulted in the wrong estimation of the conditions at which the T–O–T transition takes place. The goal of our work is to specify the boundaries of the hydrogen transition from T-site to O-site in the bcc Fe provided uniaxial compression along the [001] direction and in the absence of lattice deformation in the [100] and [010] directions.

In this work we performed density functional theory calculations within the framework of pseudopotential approach and generalized gradient approximation (GGA) of the exchange-correlation functional with Perdew–Burke–Ernzerhof form using the Quantum Espresso Package. Hydrogen transition from T-site to O-site is being observed after uniaxial compression of the lattice along the [001] direction by more than 14% without distortions along the [100] and [010] directions. This result disproves the conclusion of the transition absence in the area of small biaxial tensions in the range from 0 to 6% and biaxial compression in the range from 0 to 4% made previously in the work [1]. It also specifies theoretical data on T–O–T transition.

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Electrical resistivity and thermal conductivity of liquid aluminum in the two-temperature state

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We present calculation of the electrical resistivity and thermal conductivity of liquid aluminum in the state, characteristic for the initial stage of the interaction of femtosecond laser irradiation with metals. In this state the temperature of electrons differs from the ion temperature. It often occurs in the molten metals. We have calculated the structural factor of liquid aluminum with the help of the quantum molecular dynamics and used the Ziman approach for the calculation of the electron–ion collision frequencies. Electrical resistivity and thermal conductivity obtained agree well with

those received by the use of the combination of quantum molecular dynamics, density functional theory and Kubo–Greenwood approach [1–3]. Work was supported by the Russian Foundation for Basic Research (grant 16-02-00864) and program of the Presidium RAS "Thermophysics of high energy densities".

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Thermoelectric properties of lead telluride from first principles

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Thermoelectric (TE) materials provide direct way to convert heat to electricity. The great advantage of direct conversion method is the absence of moving parts and all corresponding issues, such as wear, noise, etc. Unfortunately, state-of-the-art TE materials have conversion efficiency of about several percents, and can not compete with traditional non-direct conversion methods. So, it is worth to search for a new TE materials with higher efficiency. The modeling is of great importance in such a challenge.

TE properties of lead telluride were obtained in Boltzmann approximation with "first-principles" electronic structure. Super-cell model of doping was used to study Na- and Tl-doping of PbTe. It was obtained that doping level of about 1.56 at. % leads to changes in electronic structure near valence band edge, and in the case of Tl doping the changes are more noticeable. As a result, Seebeck coefficient is lowered in comparison with the results of rigid bands approximation. However, Seebeck coefficient in the case of Tl doping was not found to be higher than in the case of Na-doping. Therefore, with approximations used, direct relation between distortion in the electronic density of states and increasing in the TE properties was not observed.

Calculation of thermodynamic properties of the nonideal plasmas using classical and wave packet molecular dynamics

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In this work we report on evaluation of different simulations methods for studying electron–ion non-ideal plasmas or warm dense matter. As a test system we consider the hydrogen plasma in the temperature range of $T = 2 \times 10^4$–5×10^5 K and the non-ideality parameter values $\Gamma = 0.01$–6. The internal energy and pressure are calculated using the classical molecular dynamics (MD), the wave packet molecular dynamics (WPMD) and wave packet Monte-Carlo (WPMC) [1]. Constraining boundary conditions with a harmonic wall potential are used for wave packets to prevent wavepacket spreading [2]. The self-consistency of this approach is discussed. The second result is concerned with determination of the area of applicability of the classical MD within the above mentioned parameter range. We compare the equation of state obtained by MD with the Path Integral Monte Carlo (PIMC) [3] simulations and show that at certain plasma parameters the MD method fails due to appearance of unphysical ordered structures of particles. This turns out to be the effect of the non-Coulombic pseudopotential (both in electron–electron and ion–electron interactions).

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Thermodynamic properties of quantum particles in the confined wave packet molecular dynamics model

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The methods of wave packet molecular dynamics (WPMD) and wave packet Monte Carlo (WPMC) are candidates for fast numerical description of warm dense matter and non-ideal plasmas taking quantum uncertainty and degeneration effects into account. However, the quality of thermodynamic property prediction by these methods for an extended medium remains an open question. The original quantum system in WPMD is mapped to the classical one which has more artificial "classical" degrees of freedom than the original system. It was shown previously, that for a harmonic confinement the WPMD method specially eqilibrated by a collisional thermostat serves as a good model of a quantum NVT ensemble, whereas the WPMC method samples a classical ensemble of states. In this work we study the system of quantum particles in a three-dimensional confinement with harmonic potential walls and flat floor described by WPMD. We show that for a weakly interacting system the specific heat vanishes at at low excitation energies which manifests quantum behavior. For weakly interacting system we also demonstrate quantum distribution of the system by the reference planewave eigenstates according to the temperature. We show, that the Monte Carlo method with given temperature largely overestimates the system excitation. Thermodynamic properties of interacting systems (non-ideal plasmas) are analyzed and compared to the results obtained by Path Integral Monte Carlo. Deviations and WPMD applicability ranges are discussed.

Ion-correlative model of dense mixture plasmas: Structural and thermodynamical properties

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Using the modificated model of C. E. Starrett and D. Saumon [1] we give a description of the interrelation between an ion microstructure of warm dense matter and its thermodynamical functions. We use a formalism of the cluster expansion for the Helmhotz free energy [2]. So, the pseudoatom molecular dynamics simulations [3] for the spatial ionic configurations finding are not needed. The thermodynamically consistent equations of state (EOS) with a realistically description of Coulombic features can be constructed by means of numerical differentiation. An ion microstructure can be characterized with the help of spherically symmetric radial distribution functions (RDFs). Ion–ion RDFs are obtained from the numerical solution of the Ornstein–Zernike (OZ) set of equations with the hypernetted chain closure [4]. We compute an effective interionic potentials as in [1] and use them in the OZ set of equations. An electronic subsystem of the plasmas is considered in the Thomas–Fermi–Dirac approximation with a self-consistent description for any ion-correlative effects.

All ion–ion RDFs are in close agreement with the X-ray scattering experimental data [5]. With EOS data obtained Hugoniots curves and other thermodynamical functions are analysed.

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The Hugoniot adiabat of crystalline copper based on molecular dynamics simulation and semi-empirical equation of state

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The molecular dynamics (MD) method was used for prediction of properties of copper under shock-wave compression and clarification of the melting region of crystal copper. The embedded atom potential was used for the interatomic interaction [1]. Parameters of Hugonoit adiabats (HA) of solid and liquid phases of copper calculated by the semi-empirical Gruneisen equation of state (EOS) are consistent with the results of MD simulations and experimental data. MD simulation allows to visualize the structure of cooper on the atomistic level. The analysis of the radial distribution function and the standard deviation by MD modeling allows to predict the melting area behind the shock wave front. Estimated parameters of the isotropic HA are lower than characteristics obtained in view of the crystallographic orientation. Nevertheless, the final equilibrium state of compression parameters for different crystallographic directions are close to equilibrium values at the isotropic HA.
Estimated parameters of the isotropic Hugoniot adiabatic are a little lower than characteristics obtained in view of the crystallographic orientation. The melting parameters of copper based MD simulations are consistent with [2]. These MD simulation data are required to verify the wide-range EOS of metals [3].

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The method of molecular dynamics in the description of n-alkane using atomistic modeling method TRAPPE-EH

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The Transferable Potentials for Phase Equilibria–Explicit Hydrogen method (TRAPPE-EH) means that everyone is considered atom of hydrogenium and carbon atom in the form of the separate power centers [1]. The behavior of gas condensate liquid of n-pentane was investigated at various variations of density of system and temperature by means of a method of molecular dynamics.
The equilibrium system liquid–vapour is considered. During researches of our model dependencies of pressure of our system on temperature in the range of 293–430 K were obtained. The profile pressure of system of n-pentane and density profile is constructed. Value of density of n-pentane was theoretically received. Thermodynamic functions of system are calculated. It is planned to describe in more detail an equation of state and to calculate gas condensate transport coefficients, coefficients of compressibility.
Simulations are performed using the LAMMPS MD software. The work is supported by grant No. 14-50-00124 of the Russian Science Foundation.

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Forcefield testing for molecular dynamics calculation of hydrocarbon phase diagrams

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Molecular dynamics simulations are performed to calculate vapor–liquid equilibrium of hydrocarbons and their mixtures. Three models are tested: TraPPE-UA united-atom forcefield [1], OPLS-AA [2, 3] and TraPPE-EH [4] all-atom forcefields.
The forcefields show good agreement with experimental vaporization curves of pure hydrocarbons. They also reproduce well the composition of liquid phase in binary mixtures as a function of pressure at isotherms, while some discrepancies from experimental data are observed in the saturated vapor compositions. The TraPPE forcefields show better agreement with experimental vapor-liquid equilibrium data than OPLS.
The effects of porosity on mixture phase diagram are qualitatively studied. The saturation curves in slit pores with Lennard-Jones walls are calculated. It is shown that nanopores may shift the coexistence curve. At certain wall-molecule interaction parameters, a significant widening of the pressure range of the retrograde condensation is found.
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Structures of warm dense hydrogen and liquid selenium at phase transitions

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Structure changes in selenium (warm dense hydrogen) at first-order liquid–liquid (fluid–fluid) phase transition are analyzed. The calculations are made in framework of DFT, using program package VASP. Liquid selenium consists of chains that get destroyed with the rise of temperature and pressure. The chain length along isotherms crossing phase coexistence line are defined and analyzed. The definition of bond between two atoms is taken geometrically; two atoms are bonded if distance between them is less than predefined r_c. It is possible to take r_c as first maximum or first minimum of pair correlation function. Not only chains but more complex structures (e. g. cycles, branching) are constructed. To deal with them, it is necessary to specify the concept of chain. The simple way is not to differ between chains and more complex structures, considering chain length as number of atoms of such structure. Another approach is to define chain as a sequence of two-fold atoms ending with one-fold or three-fold atom. The similar analysis is conducted for warm dense hydrogen, where pairs and cycles of three atoms with different bond length are expected. The bond lifetime and correlation between atoms depending on interatomic distance is also calculated. The work is supported by the RSF grant No. 14-50-00124.

Atomistic simulation of defects behavior and phase transitions in pure Zr and Zr–Nb alloy

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We report a new attempt to study properties of Zr–Nb structural alloys. For this purpose we constructed an angular-dependent many-body interatomic potential. The potential functions were fitted towards the *ab initio* data computed for a large set of reference structures. The fitting procedure is described, and its accuracy is discussed. We show that the structure and properties of all Nb and Zr phases existing in the Zr–Nb binary system are reproduced with a good accuracy. The interatomic potential is appropriate for study of high-pressure hexagonal ω-phase of Zr. We also estimated characteristics of the point defects in α-Zr, β-Zr and Nb, results are proven to correlate with the existing experimental and theoretical data. In case of α-Zr the model reveals anisotropy of the vacancy diffusion, in agreement with previous calculations and experiments. The potential provides an opportunity for simulation of Zr–Nb alloys based on α-Zr and β-Zr. This conclusion is illustrated by the results obtained for the alloys with different niobium concentrations: up to 7% in case of hcp alloys and up to 50% for bcc alloys.

The investigation of the recrystallization process in the Zr–Nb alloys

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The Zr–Nb alloys are widely used in the development of modern structural materials. Thus, the alloys based on the HCP-zirconium with the Nb concentration about 1–2.5%, are one of the main materials for the manufacture of structural elements of the Russian nuclear reactors. In addition, the study of the bcc Zr–Nb alloys with the Nb fraction of 20–40% finds application in problems of biomedical materials. It is known that zirconium-niobium alloys can be transformed into a nanostructured state with a characteristic grain size of 10 to 100 nm. Such a structure makes different phenomena possible at thermal, deformation, radiation and other exposures. Recrystallization is the process of thermoactivation of the growth of average grain size by reducing some of the grains and growth of others. In general, the average grain size at a given temperature is influenced by the following factors: concentration of the component of the alloy, the initial grain size, heating rate, and voltage, which is alloy.
In our work the recrystallization is studied using computer simulations. For the bcc-alloys of the Zr-Nb, the contents of the Nb are varied from 10 to 40%, for hcp—from 1 to 6%. The following parameters are obtained for the different temperatures and contents: the energy of the grains' edge migration—using the molecular dynamics method; the dependencies of the average grain size from time—using the phase field method. In particular, it can be concluded, to what extent, the concentrations of Nb and Ti influence the termination of the grain growth.

Atomistic simulations of phase and structure transitions and defects formation at swift heavy ion irradiation in uranium–molybdenum alloy

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U–Mo alloys are the most prominent candidates for advanced fast-neutron reactors due to high thermal conductivity, low thermal expansion, and high melting point.
Phase and structure transitions and mechanisms of the stabilization of homogeneous cubic structure are important for describing the evolution of the nuclear fuel in the operating conditions and fuel fabrication. Structural properties of cubic and tetragonal phases of U–Mo alloys are studied using atomistic simulations. For pure uranium and U–Mo alloys at low temperatures body-centered tetragonal structure (bct) is observed, which is similar to the metastable γ^0-phase found in the experiments. At higher temperatures bct structure transforms to a quasi body-centered cubic phase.
Another mechanism of phase and structure transitions is swift heavy ions (SHI) irradiation. High energy transfer into the electronic subsystem and relaxations processes lead to the formation of structural defects and cause specific effects, such as the track formation. Defects formation and structure transitions in U–Mo alloys at irradiation of SHI has been carried out using the two-temperature atomistic model. It is shown that defects formation may be produced without melting and subsequent crystallization. Threshold stopping power of SHI for the defects formation at irradiation in the various conditions are calculated.

Progress in developing a multi-scale plasticity model for oxide nuclear fuel

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A multi-scale modelling approach develops an hierarchy of computational methods, uses them to produce qualitative and quantitative output at specific spatial and temporal scales, and then combines their results together to gain an in-depth understanding of a specific complex process (e.g., plastic deformation in solids). We report recent progress in developing one such model to study plasticity in uranium dioxide. Although very simple, currently combining only two methods: classical molecular dynamics and two-dimensional discrete dislocation dynamics—this model was recently used to describe the dynamics of an entire dislocations ensemble with a specific mobility function evaluated using atomistic simulation. In the accompanying presentation a detailed discussion of the dislocation mobility evaluation procedure will be given together with a brief description of how one may convert molecular dynamics (MD) data to an analytical expression for the glide mobility. Details of incorporating this function into a higher scale simulation will also be mentioned. Finally, we will present the results of our on-going development of the two-dimensional dislocation dynamics code and point out new predictive capabilities now available with the use of atomistic input. This work was supported by the Russian Foundation of Basic Research, grant No. 16-38-60016.

Study of phase transition in the pure metal melt during ultrafast cooling by method of higher-order correlation functions

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This paper discusses results of the application method [1] of spatial correlation functions on glass-forming liquid of pure metal melt, by performing molecular dynamics simulations. We define high-order correlation function that quantifies the spatial correlation of single-particle displacements in liquids and amorphous systems. The dependencies of the different 4-point spatial functions [2] on velocity of ultrafast cooling and type of material are given. Other criteria of phase transition were discussed in [3]. In addition, we analyze differences between models and finding out how to choose proper criteria for real temperature of phase transition.

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Anisotropic thermal expansion of high explosive crystals under atmospheric pressure

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Thermal expansion (compression) is characteristic of practically all materials. Note that temperature induces different response in each material (expand, compress or oscillate), and thus undergo polymorphous transitions with the change of all properties, etc. Moreover, response of structure fragments in the same material in different directions turns out to be individual. So, studying the process of anisotropic thermal expansion (compression) of crystalline explosive materials presents some features of interest and approaches us to the detailed understanding what the nature of their structure is. In turn, the data given by the investigation into the thermal expansion of high explosive (HE) crystals can be used to derive equations of state and also to analyze processes of HE processing. The X-ray diffraction experiment at final temperatures is presented to determine the state of certain crystalline explosives, i.e. TATB, BTF, HMX, PETN, and RDX. These HE were processed and the paper presents functional relationships how parameters of the HE crystal structure are changing under certain temperatures in quasi-isobaric conditions ($P = P_{\mathrm{atm}}$) within the entire range of HE crystals existence in the condensed state. The powder X-ray diffraction analysis (PXRD-analysis) performed with the help of the diffractometric station determined parameters of the crystalline structure, i.e. cell metrics, lattice constants, elementary volume, density, and substructure sizes. The full-profile analysis was used for processing with the regard for force interactions "atom–atom".

Oscillation and parameters phase equilibrium ammonium perchlorate crystals in the polymorphic transition region

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Polymorphism of crystalline materials is a part of their structural-phase changes at any type (thermal, baric *etc.*) of impacts. There are at least two known types of polymorphic transitions, i.e. enantiotropic and monotropic. Currently, ammonium perchlorate (AP) is revealed to have the polymorphous transition of the first kind within 511–517 K and the data on the isotropic change of thermal expansion coefficients in the pressed AP are analyzed. Qualitative results on the changes in the diffraction pattern of X-rays reflected from crystals are obtained to perform detailed analysis of the polymorphous transition in AP under atmospheric pressure. The structure of AP crystals at final temperatures was thoroughly investigated with the help of the X-ray diffractometer within 150 and 550 K with the 10 increment. Changes recorded in the diffraction pattern indicate changes in the crystalline structure, phase composition, and oscillation of the structural state in AP. Crystallographic models of two modifications of AP, i.e. orthorombic and cubic, are developed to perform precise, standard-free phase and structural analyses. The full-profile analysis (quantum simulation combined with the differential Fourier-transforms) used to process X-ray patterns. So, the polymorphous transition is proved to be incomplete in AP under atmospheric pressure up to the time of its complete decomposition. A simple exponential model is proposed for description of the phase equilibrium process in AP.

On the role of heat flux in the non-stationary thermal problems

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One of the main notions of classical irreversible thermodynamics is the local entropy rate of production $p = \sum F_j J_i$, which is a bilinear function of forces F_j and fluxes J_i, whereas in the linear regime it is assumed that the fluxes are linearly dependent on forces $J_i = \sum_j L_{ij} F_j$, where L_{ij} are the phenomenological coefficients. For steady-state one-dimensional heat problem ($\partial T/\partial \tau = 0$), where the temperature is only a function of a single spatial coordinate $T(x)$, it is known, that force $F_j(x)$ generates the corresponding in value heat flux. We consider an opposite case—one-dimensional non-stationary change of temperature $\partial T(\tau)/\partial \tau \neq 0$ with the absent gradient of temperature $T \neq f(x)$. Under these conditions, we are interested to investigate the behavior of local entropy rate of production $p(\tau)$ and its components $F_j(\tau)$, $J_i(\tau)$ over time. Basis is the analysis of experimental thermogram obtained in the process of instant cooling of a spherical solid-phase molybdenum sample. We show the results of computational modeling, proving that the isothermal approximation holds along the radius of the spherical sample: this proof is necessary to determine the entropy density $s = S/V$ (where S—the entropy, V—volume of a sphere). Then we describe the method to determine the dependency of local entropy rate of production, force and heat flux on time. It has appeared, that during cooling the solid sphere from molybdenum the local entropy rate of production and heat flux have identical dependence from time-aspire to a minimum with zero value at approach an ambient temperature (thermodynamic extremum principle). It has allowed draw a conclusion that in a considered non-stationary problem the heat flux plays defining role unlike a stationary one-dimensional problem in which force (a gradient of temperature) is an original cause, and the heat flux results from action of force.

Laser vaporization mass spectrometry of ZrC_x at temperatures up to 4400 K

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Zirconium carbide evaporation was studied using high-speed mass spectrometry coupled with laser-induced evaporation up to extremely high temperatures. The temperature limit (3000 K) of conventional techniques (Knudsen cell evaporation [1, 2]) was significantly overcome. The current technique is the further extension of one recently developed earlier in [3] for studying of graphite sublimation and uranium dioxide evaporation up to 4100 K. Therefore a measuring procedure and an experimental set-up were developed in order to reach significantly higher temperatures.
In present work the vapor composition of zirconium carbide was examined at temperatures much above the solidus line, i.e. at vaporization of two-phase or liquid ZrC_x. Time-of-flight mass spectrometry and fast pyrometry enabled measurements of temperature dependence of vapor composition. Samples of various compositions ZrC_x (x between 0.65 and 1.0) were investigated. Relative partial pressures of C_1–C_3 molecules, zirconium isotopes, ZrC, ZrC_2 and Zr_2C species were obtained. Measured evaporation enthalpy of zirconium over liquid ZrC is amounted to 720 kJ/mol K. The C/Zr ratio was shown to decrease greatly with the temperature from the value of 10 to less than 0.5 for stoichiometric zirconium carbide. It was found that the C/Zr ratio changes slightly approaching the value of less than 0.2 for the samples within the homogeneity domain of zirconium carbide.

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The structural-surface analysis of carbon black properties obtained by method of laser evaporation of graphite

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This work is devoted to a new way of obtaining carbon nanodisperse powders—carbon blacks, having in advance set properties, for application in electrochemical devices: porous electrodes of supercapacitors, fuel cells *etc.*

The complex of requirements to carbon blacks for electrochemical applications is rather extensive and significantly depends on specific electrochemical devices in which it is planned to be used. Thus, success of use of carbon black in electrochemical devices in many respects depends on an opportunity to manage its physical and chemical properties during synthesis. At the same time it is important to note that production of the Russian detonation carbon black suitable for electrochemical devices is stopped now. Dependence on foreign suppliers of carbon blacks strongly complicates projects implementation on production of innovative sources of current.

In this work, the developed method of receipt of disperse carbon materials by method of laser heating of graphite samples is described. Results of a research of their physical and chemical properties are provided. The main difference of the offered method from traditional one consists in use as graphite raw materials, but not hydrocarbons. Carbon black obtained thus differs in the high content of carbon (more than 99%) and has the high specific surface.

Recent advances in laser-pulse melting of graphite at high pressure

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Melting temperature of graphite and nature of liquid carbon remains a subject of permanent discussions in the literature for many decades. The main reason of this inconsistency is the extremely high melting temperature of graphite making it the most refractory material. The present study deals with a further improvement of the laser-heating technique with the aim to reach a higher reproducibility of the results, to improve and to broaden means of optical measurements and to better control the process of cooling and freezing of liquid carbon. The important aspect of this work is to study the nature of the cusp on the thermogram in the melting region. Unlike to other materials, the heating rate in liquid higher than in solid state. Understanding this phenomenon may help to investigate the changes of thermal conductivity between solid carbon and liquid in wide pressure range. The melting thermogram was obtained for isotropic graphite at pressures 0.5–6 kbar. Another important aspect of this study is crystallization of liquid carbon. Visualization of liquid phase was made by high-speed camera. To reduce the influence of thermal radiation the interference filter was mount in the camera optics and the sample surface was lighted by diode laser with optical power 100 W. Analysis of solidified liquid carbon and vapor condensate was made by scanning electron microscope.

Experimental investigation of thermal expansion of graphite at high temperatures

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Using the experimental setup for investigation of the thermophysical properties of refractory materials under high pressure and temperature [1] a few experiments with pyrolytic graphite were carried out. Experimental data on the linear thermal expansion in the perpendicular and parallel to the basal plane direction were obtained. Change of volume during the heating up to the melting point was equal to $\Delta V/V_0 = 1.21$.

Our approach allows adjusting the heating rate in a wide range from 10^6 to 10^7 Ks^{-1} at a high static pressure of the surrounding gas up to 1 kbar. Temperature $T(t)$ is measured by special two-channel optical pyrometer. Beside that current $I(t)$ and voltage drop $e(t)$ across the potential probes in the central part of the specimen during the experiment are determined. For the measurement of thermal expansion $\Delta L(t)$ of material a technique based on the thermal radiation images of the hot specimen was used.

The results obtained allow calculating the density of pyrolytic graphite in the wide range of high temperatures up to the melting point and in the two-phase region.

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Experimental investigation of thermophysical properties of eutectic $ReC_{0.3}$ at high temperatures

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Using the experimental setup for investigation of the thermophysical properties of refractory materials under high pressure and temperature a few experiments with eutectic rhenium–carbon system were carried out. Experimental data on the specific enthalpy, heat capacity, electrical resistivity and heat of melting of $ReC_{0.3}$ were obtained. Our approach allows adjusting the heating rate in a wide range from 10^6 to 10^7 Ks^{-1} at a high static pressure of the surrounding gas up to 1 kbar. By measuring the surface temperature of the specimen during the experiment $T(t)$, current $I(t)$ and voltage drop $e(t)$ across the potential probes in the central part of the specimen during the experiment, one can determine temperature dependence of enthalpy $H_P(T)$, specific heat capacity $C_P(T)$ and the other properties of the material [1].

Dependencies of the specific heat capacity and enthalpy of the eutectic $ReC_{0.3}$ obtained in the experiments are in a reasonable accordance with the estimates based on the Kopp–Neumann law. The value of electrical resistance of $ReC_{0.3}$ and heat of fusion of this material were for the first time obtained. Because of its absence the literature data for the eutectic composition in the entire temperature range and, for the stoichiometric composition, near the melting point are of great interest, particularly in the context of using of melting points of refractory carbides as high temperature reference points and, for some of them, in high-temperature engineering.

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Thermal stability comparison of micro and nano diamonds produced by detonation

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Micro and nano diamonds can be obtained as the explosion products. Used carbon explosives have the negative oxygen balance. Microdiamonds are formed by detonation in the water environment and nanodiamonds are obtained in the air one. It's well known that properties of small particle depends on the size [1]. Thus, the task of the thermal properties comparison of the detonation micro (DMD) and nano diamonds (DND) is represented continuous interest. The comparison of the DMD and DND is carried out by method synchronous thermal analysis in the Netzsch STA 409 PC. Annealing of samples was conducted in a closed corundum crucible (Al_2O_3) at atmospheric pressure of argon flow. Heating conditions are from room temperature to 800, 1200, 1500 °C at rates 2 and 10 K/min. As a result of this work the thermal and structural properties of micro- and nanodiamonds were compared. Experimental with microdiamond is more reproducible. It was shown that DND transit to the amorphous state is higher 500 °C [2, 3]. While the microdiamonds are stable even at 1500 °C. In this work it was showed the influence of the heating rate on particles sizes of DND and DMD powders. In the case of annealing nanodiamonds the planar carbon structure was observed.

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Heat transfer under high-power heating of liquids: An experience of monitoring of oils

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The significant experience of investigations of liquids quality by the method of controlled pulse heating of a wire probe has been accumulated. The pulse duration was varied in the range of 1–15 ms. A region of probe temperature rise was limited from above by the value of spontaneous boiling-up temperature of a substance. The objects of study were turbine oils, transformer oils, hydrocarbons. The water content was varied in the range from 10 ppm (initial sample) to 350 ppm (watered sample). A sharp increase in the heat transfer intensity for watered sample with respect to that of initial one has been revealed. The observed effect was manifested solely at temperatures close to the values of boiling-up temperature of watered sample.
The study was partially supported by the Russian Foundation for Basic Research, research project No. 16-08-00381-a.

Heat transfer at high-power heating of water in supercritical region

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The aims of our report were defined as follows: (i) to elucidate the characteristic features of supercritical heat transfer, which accompanies the high-power heat release in a compressed liquid, and (ii)

to provide the experimental justification for selecting the operating pressure of supercritical water (SCW) for industrial heat transfer equipment, including mini-sized heat exchangers.
Application of short-term techniques for studying the supercritical heat transfer allowed the authors to obtain new interesting results. Within this approach, the impact of the two main factors (namely, convection and gravity) complicating the study of heat conduction in SCW proved to be almost eliminated. As a result, the effect of threshold decrease in the heat transfer intensity was revealed in course of a fast transition from compressed liquid to supercritical fluid state along the isobar.
Data obtained in the pulse experiments gave ground for the assumption that under conditions of high heat flux densities, thermal resistance of the boundary layer of supercritical fluid is a limiting factor for heat transfer. The stronger the impact of this factor is expressed, the closer the pressure value to critical pressure. In this context, with respect to the application of SCW as a coolant, the expansion of the region of variation of supercritical pressure values in the experiments towards their increase appears to be timely.
The study was supported by the Comprehensive program of the Ural Branch of RAS, research project No. 15-20-2-18.

Measuring the surface tension and critical wetting angles of indium and tin microdroplets with a transmission electron microscope

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It is well known that ultra-fine system, due to the high specific surface area, have significant excess surface free energy, which makes them inherently unstable [1]. Thermophysical properties of nanoparticles have a pronounced size dependence that must be considered in the design of structural nanomaterials [2]. In this regard,

experimental and theoretical study of size effects is an important and urgent task. In this study we discuss the features of capillary properties of microdroplets fusible metals, which are used for the study of a transmission electron microscope [3]. Measurements of contact angles have been performed using microscopic images obtained with a transmission electron microscope. As an example the measurement procedure have been illustrated on indium and tin microdroplets.

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Berezinskii–Kosterlitz–Thouless and Vogel–Fulcher–Tammann criticality in XY model

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Celebrated Berezinskii–Kosterlitz–Thouless (BKT) works brought a new seminal paradigm of topological phase transitions driven by topological defects. Among many remarkable unique properties of the BKT transition, the singularity of its critical behaviour stands out. On approach from above to a critical temperature, T_{BKT}, the correlation length diverges extremely rapidly,

$$\xi \sim \exp[\sqrt{E_0/(T - T_{\mathrm{BKT}})}],$$

much faster than any power law governing correlation length $\xi \sim |T - T_c|^{-\nu}$ for a standard continuous phase transition. This strikingly

resembles the manifest criticality of a glass transition where correlation length obeys the famous Vogel–Fulcher–Tammann (VFT) law, $\xi \sim \exp[E_0'/(T - T_G)]$, and posits a question about the deep interconnection between the two. We develop a gauge theory of the topological defects driven phase transition in the weakly disordered XY model, the harbor of the BKT physics. We find that while in two-dimensions the liquid of topological defects freezes according to the BKT scenario, the three-dimensional topological liquid exhibits more singular VFT criticality signaling freezing into a nonergodic glassy state. Our findings unravel the nature of a glass transition as a topological phase transition.

Quantum nuclear effects in water using centroid molecular dynamics method

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Quantum nuclear effects can play a major role in prediction of equation of state and transport properties of matter. The examples of such systems are water and liquid hydrogen at low temperatures. In these cases, the behavior of hydrogen atoms is quantum and classical molecular dynamics (MD) could not be applied [1].
We study quantum effects in water using path integral molecular dynamics method. The centroid molecular dynamics (CMD) [2] realization of this method is used. In CMD, the quantum nature of atom is presented by a lot of replicas that interact with each other via harmonic potential. The final Hamiltonian of the particle has a form:

$$H_n(\mathbf{q},\mathbf{p}) = \sum_1^n \Big[\frac{\mathbf{p}_k^2}{2m} + \frac{m\omega_n^2}{2}(\mathbf{q}_k - \mathbf{q}_{k+1})^2 + V(q_k)\Big].$$

The quantum properties of system are calculated: gyration radii of the atoms, velocity autocorrelation functions and radial distribution functions. The interaction potential q-TIP4P/F is used [3]. Diffusion coefficients are obtained using Green–Kubo method. The results calculated in CMD are compared with classical MD and the quantum effects are analyzed. The work is verified with [3]. The temperature influence is also treated.
The study has been funded by the Russian Academic Excellence Project "5-100".

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Nanostructures nucleation in carbon–metal gaseous phase: A molecular dynamics study

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We apply molecular dynamics methods for describing the nucleation of carbon nanostructures. For the accurate description of the nucleation process at the nano scale we use reactive potentials which take into account the breaking and the formation of bonds using the chemical concept of the bond order.
In the work [1] the homogeneous nucleation of carbon nanostructures from the gas phase was simulated with reactive potentials ReaxFF [2] and AIREBO [3]. Our results have shown that nucleation in the AIREBO model is going more actively than in the ReaxFF one. Here we argue that AIREBO provides more accurate description of condensed carbon and use the new variant of ReaxFF [4] that is consistent with the AIREBO model.

In this work we consider nucleation in two component gaseous phase with carbon and metal atoms. We quantify the degree of nucleation acceleration (catalysis) that metal atoms (e.g. iron) introduce for the growth of carbon–metal nanostructures.
The work is supported by Russian Science Foundation (grant 14-50-00124).

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Sticking coefficient for Fe cluster growth

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Molecular dynamics method is used to study Fe cluster growth. First, the cluster is created and heated to the temperature needed. Finnis–Sinclair potential [1] is used for interactions between atoms of the cluster. Then, incident atom coordinates and velocity are defined. The velocity is chosen randomly using the Maxwell distribution for a room temperature. The incident atom interacts with the cluster through the Lennard-Jones potential [2]. The aims of this work are calculating sticking coefficient, detachment coefficient and cluster growth rate. For now, sticking coefficient is calculated for a number of temperatures between 300 and 2500 K and several sizes of the cluster. The fact of sticking is defined both geometrically and energetically. Incident atom belongs to the cluster if the distance between the atom and the cluster is smaller than a cutoff radius for a period of time and the atom energy is negative. Comparison with the experiment [3] is conducted.
The work is supported by the grant No. 14-50-00124 of the Russian Science Foundation.

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Universal cluster distribution function in the system of randomly distributed particles

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Consider a system with N_0 particles which are randomly distributed with density $n = N_0/V$ inside the volume V. The mean distance between particles is $l_0 = 0.55n^{-1/3}$ [1]. We assume that two chosen particles belong to the same cluster if the distance between them does not exceed some "interaction radius" a. Then the distribution of particles over the clusters is defined by the ratio $\eta = a/l_0$. We enumerate the clusters in descending order of the number of particles in each cluster. That is, for example, $k = 1$ is the sequence number of the cluster that contains the maximum number of particles (i.e. it is a biggest cluster in the system). Let N_k to be the number of particles in a cluster with the sequence number k, i.e. $\sum_{k=1}^{N_0} N_k = N_0$. Numbers N_k define the distribution of particles over the clusters. We have evaluated these numbers by means of the Monte-Carlo simulation of random particle spatial distribution with fixed n. Each value of N_k is an average result of 50 random distributions of $N_0 \leq 10^4$ particles. The quantity $W_k = N_k/N_0$ can be considered as a probability that some particle from the system belongs to a cluster with the sequence number k. We show that for large $N_0 > 10^3$ the distribution function W_k does not depend on N_0 and is described by some universal distribution function. The shape of this function is defined by only one parameter η. The results have been compared with LAMMPS parallel computer package molecular dynamics simulation for noble gases [2].

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Graphene nanobubbles: Molecular dynamics simulation

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Two-dimensional material placed on atomically flat substrate can lead to formation of surface nanobubbles with different types of substances trapped inside. Experimental studies shows that the matter inside the nanobubbles experience extreme pressures up to 1 GPa [1–3]. Therefore phase transitions of confined substance can be expected. Using molecular dynamics, we study graphene nanobubbles with radius in range 10–40 nm with argon atoms inside. Their shapes are found to exhibit universal scaling, in agreement with experimental data and analysis based on the theory of elasticity of membranes. We also showed that the thermodynamic state of argon in the nanobubble is above the critical point. Furthermore, the inside pressure as function of the nanobubble volume is obtained. This can be used as additional verification of atomic-force microscope measurements of the graphene nanobubbles.

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Elaboration of gas–particle interaction terms in models of mechanics of multiphase media

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One of the promising approach for modeling of heterogeneous systems is continual approach of dynamics of multiphase media. It is developed in works of well known russian scientists as Rakhmatulin H. A., Nigmatulin R. I., Nikolaevskii V. N. etc. and is based on averaging of conservation laws over space. As a result we get conservation laws for averaged parameters of media which are similar to classical laws of fluid mechanics but with source terms describing interphase interactions (mass, momentum, energy). This method is good for mixtures with small concentrations of dispersed phase. Usually [1–3] these terms are taken in form of solutions of classical problems of flow around sphere of viscous fluid or impirical relations from experimental data. Averaging of parameters leads to loss of local values of functions demanded for calculating interphase interaction terms. Accounting of phase geometry is made through volume ratios of phases, what makes such models inaccurate. For creating more accurate models it is necessary to know function values and their derivatives of high orders in the averaging area. In this work on the basis of linear approximation of parameters of mixture it is shown how it can be achieved and what relations are needed to be added to classical model of ideal and viscous gas and dispersed phase of spherical particles.

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Response functions in inhomogeneous media

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The problem of studying the response of an inhomogeneous condensed medium to the external action is now extremely actual. As a rule, the first step in decision of a task is the solution of the simplified problem, and the second step in the approximate calculation of the corrections due to the small terms, discarded in a simplified task. Correction computation by perturbation theory in the present work used to determine the response function in the external weak electric field.

Density functional theory allows theoretical justification of approximate methods in the study of interatomic interactions in the molecules [1, 2], intermetallic compounds and chemisorption [3].

New results were obtained. This work, which is a continuation of [4], it is not limited to the Thomas–Fermi approximation. Polarizability determined sequentially within the bounds of statistical model taking into account of the external field in the original equation of the model. For the first time this approach was used in [5], where the test function was expressed in terms the unperturbed density and a variational parameter. Using this model, polarizability calculations for atoms with closed electron shells were carried out.

This work was supported in the framework of the base part of the Russian DES government task KBSU for years 2017–2019.

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Calculation of the equations of state for mixtures on the example of lunar soil

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Two independent approaches are used for creation of the equations of state (EOS) for mixtures of soil components. These approaches give close results.

In the first approximate approach the rule of an additivity of shock adiabatic curves of mix components is applied when calculating a resultant shock adiabatic curve. Then the calculated shock adiabatic curve of mix is taken as a basis at creation of multicomponent soil EOS. This approach is simpler for numerical realization.

In the second approach equalities of pressure and temperatures are supposed in all components of soil. The system of the nonlinear equations received as a result of this assumption is solved by numerical method of iterations for density of mix components. The second approach is more common and correct. This approach allows to create mix EOS when we known EOS of components. However, it demands bigger time losses on the computer.

The received coincidence of results at various approaches confirms applicability of the assumption about additivity of shock adiabatic curves for multicomponent lunar soil.

Thermodynamic parameters of mixture with epoxy as a component under shock wave loading

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The results of numerical experiments on modeling of shock wave loading of mixtures are obtained by using thermodynamic equilibrium components (TEC) model [1] are presented. The thermodynamic parameters are modeled for the mixtures that include epoxy as component. The important point is the possibility of phase transition of the components under shock wave loading. The significant change in volume in the region of phase transition components included in the mixtures allows us to expand the range of variation of thermodynamic parameters of the mixtures under shock wave loading. This result allows us to create purposefully the necessary conditions for the synthesis of new materials. When modeling the material in the region of phase transition is considered as mixture of low-pressure phase and high-pressure phase. This approach allows us to describe reliably the thermodynamic parameters for polymorphic phase transition [2]. Interest in the study of compressibility of such mixtures is associated with the possibility of creating materials with the required properties (high strength and heat resistant ceramics) and with the properties of the materials themselves. A good agreement of these model calculations with the data of different authors that defined on the experiments basis is obtained [3]. The present model is used for selecting the compound and the ratios between the mixture components in order to obtain the prescribed characteristics under the shock wave loading of solid and porous materials and mixtures.

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Computational modeling of porous ceramic material

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Compaction of ceramic powders using dynamic processes has been widely studied in terms of the manufacture of ceramics with unique properties and microstructures. At the same time, there are a limited number of works, which are exploring the processes of dynamic consolidation of ceramics in quantitative terms, as well as investigates the physical processes associated with long flowing. When constructing a model of the dynamic compaction of the porous material should take into account three key elements: the equation of state (EOS) to describe the dependence of the pressure–density, including a non-linear effects of sealing; yield surface, which describes the dependence of the strength of intact and damaged material, depending on the pressure and the fracture model, which describes the transition of the material from the intact in the ruined state. The change in porosity is described relations Carroll–Holt [1]. To close the system uses small number of parameters equation of state [2], which allows you to make calculations of shock-wave processes with a minimal number of physical parameters as initial data. The stress state of the material presented in the form of Johnson–Holmquist [3]. The extent of the destruction of the material is expected to accumulate by increasing the plastic deformation of ceramics by the movement of the plastic deformation, using an expression similar to the model of destruction of Johnson–Cook [4].

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Calculation of phase diagrams of binary mixtures using the equations of state of the van der Waals type

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Hydrocarbon mixtures filtration process simulation development has resulted in use of cubic equations of state of the van der Waals type to describe the thermodynamic properties of natural fluids under real thermobaric conditions [1]. Binary hydrocarbon systems allow to simulate the fluids of different types of reservoirs qualitatively, what makes it possible to carry out the experimental study of their filtration features. Exploitation of gas–condensate reservoirs shows the possibility of existence of various two-phase filtration regimes, including self-oscillatory one, which occurs under certain values of mixture composition, temperature and pressure drop [2]. Plotting of the phase diagram of the model mixture is required to determine these values. A software package to calculate the vapor-liquid equilibrium of binary systems using cubic equation of state of the van der Waals type has been created. Phase diagrams of gas–condensate model mixtures have been calculated.

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Simulation of hydrogen and deuterium storage in intercalated graphite–potassium compounds

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Graphite–potassium intercalation compounds (GPIC) have intercalated layers with a lacunar structure in which it is possible to accumulate large quantities of H_2 or D_2 molecular. The reason is that interlayer distance in GPIC is much larger then in ordinary graphite monocrystal. For an example interlayer distance in GPIC KC_{24} $d = 5.40$ Å [1], whereas in graphite it is 3.35 Å. We have full field simulation of GPIC hydrogen capacity for different structures KC_{12s} for temperatures close to the boiling point of nitrogen. Lattice dynamic for GPIC doped by hydrogen–deuterium atoms have been studied in frame our approach.

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Cavitation bubble dynamics in viscous liquid and fusion

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An analytical approach developing in our previous paper [1] for viscous droplets have been extended of the case of gas bubble immersed in viscous liquid. A method for filling the bubble by gaseous deuterium and deuterium–tritium mixture is proposed. The achievable pressures and temperatures during bubble collapse processes for a given external pressure are calculated. The neutron flux due to fusion reaction is estimated and compared with the results of work [2].

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The viscosity behavior at the glass transition process

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Molecular dynamics study of shear viscosity behavior of liquid Al is performed. The embedded atom method potential is used at the simulation of isobaric cooling [1]. The viscosity is calculated using the Green–Kubo formula.

The dependence of kinematic viscosity on temperature during the glass transition process is presented. The viscosity values above the melting temperature are close to the available experimental data [2]. The ensemble-averaged and time-averaged stress autocorrelation functions (SACFs) are obtained in the temperature range 300–1200 K. The asymptotic behavior of SACFs is considered. At short times there are two exponential decay parts. At large times, the exponential decay changes to a power-law decay. The dependence of the SACF relaxation exponent on temperature is obtained. It was found, that the glass transition criteria [3, 4] are related to the steep decrease of the value of the decay exponent of the SACF.
Also, the hysteresis of the transport coefficients is analyzed.
The work is supported by the Russian Academic Excellence Project "5-100".

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Influence of the composition on dynamics of ions and microhardness of chalcogenide glasses

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Influence of the composition on microhardness and parameters, which define dynamics of silver mobile ions in chalcogenide $AgGe_{1+x}As_{1-x}S_3$ have been analyzed. From the values of microhardness, which was measured using microhardness tester HVS-1000A, we concluded that with the increasing concentration of germanium, microhardness increases as well. The reason of it could be the existence of high-energy connections Ge–S and it shows that the

number of these connections grows [1]. Values of parameters, which define dynamics of ions, such as the mean-squared displacement, were obtained using linear-response theory and Kubo formulas [2] from the electrical conductivity spectra, which was measured in a broad frequency range by impedance spectroscopy. The results we got for different concentrations of germanium in samples correlate with the values of microhardness.
The researches were supported by Russian Foundation for Basic Research grant No. 16-02-00857-a.

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Deformation and breakup of composite droplets in the narrow channel under shear flow: Numerical simulation

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The hydrodynamic properties of the composite droplets comprised of a single core and shell are reported. Such objects take advantage in manifold applications including energetics, material science, medicine, biology, pharmaceutics, microuidic technologies, etc. Most of them require knowledge on deformation and ultimate behavior of the systems under various flow conditions. In this communication, the attention is focused on studying effects of the channel walls on the mechanical properties of the 3D composite droplets under simple shear flow condition. By means of numerical simulations, it was found that unlike the broad channel, the simple shear flow in

the narrow one leads to a significant increase in droplet elongation. The particular results are sensitive to the set of parameters as ratio of the core to shell radii, ratio of the outer droplet diameter to the distance between the solid walls (confinement parameter), and ratios of viscosities of core, shell, and continuous fluids. The critical capillary numbers at breakup along with peculiarities of defragmentation of composite droplets of different compositions and viscous properties were revealed for the first time.

The generation of microdroplets in the co-flowing Newtonian and non-Newtonian fluids: Mathematical modeling

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Production of monodisperse emulsions and polymeric microparticles is of great importance for a number of applications as photonic crystals, energetics, microbiology, drug delivery system, etc. One of the efficient ways of generation of monodisperse microdroplets is a co-flow of two immiscible liquids through the coaxial capillaries. The resulted droplet sizes are sensitive to capillary flow rates, viscosity ratios of continuous and dispersed phases. In this study we investigated numerically an influence of rheological properties of the continuous phase to peculiarities of droplet formation in the dripping and jetting modes. As a dispersed phase we considered Newtonian liquid injected into the shear thinning (polymeric) fluid flowing through the outer capillary. The shear rate dependence of viscosity of this fluid was described by the Carreau–Yasuda model. We found that in this case the dripping and jetting modes are shifted towards the larger flow rates of the continuous phases while the

droplet size grows as compared with the corresponding Newtonian fluids.

Implementation of low-background isotope markers method for the checking of graphite–potassium intercalation efficiency

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This paper presents results on low-background gamma activity measurements of graphite–potassium intercalated samples. Low-background gamma-spectrometer 4 HPGe [1] placed in NIKA chamber of Baksan neutrino observatory made possible to establish the amount of potassium embedded in the graphite lattice in processes of electrochemical intercalation from saturated aqueous with natural (0.012%) abundance of isotop K40. The number of K40 decays for 384 hours graphite–potassium intercalated sample exposure was $N_1 = 768$, which corresponds to about one milligram of potassium atoms in graphite lattice. The signal to background ratio is equal to 45.

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Equation of state calculation for Ar and water with the application of fractional order derivatives

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In the continuation to our resent works data [1–3] we present the generalization of thermodynamics in formalism of fractional derivatives with the calculation of the one-parametric "fractal" state equation with second virial coefficient for argon and water.
The results of our calculations are in satisfactory agreement with the experimentally measured data. In addition, it is possible to extrapolate the equation of state to the extreme thermodynamic parameters, where experiments are difficult or impossible. Thus, the thermodynamics of fractional calculus, containing a traditional thermodynamics (which is based on the principle of local equilibrium) as a special case, is expanding its scope, encompassing the processes under fulfillment of the principle of local non-equilibrium.
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Thermodynamic properties of the argon dimers Ar_2^+ and Ar_2

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The compounds containing the ions of argon play a essential role in the mass spectrometry with argon plasma sources. It is required to know, how these ions influence final measurements. However, the thermodynamic properties of such molecules as the argon dimer and its ion or 3d metal argide ions have not been studied sufficiently. In the previous work we calculated the internal partition functions and thermodynamic properties for VAr^+ and $CoAr^+$ [1]. In this work we performed accurate calculations of the internal partition functions for the ionized and neutral argon dimers Ar_2^+ and Ar_2. Using the molecular constants (mainly from [2] for Ar_2^+ and [3] for Ar_2), we performed calculation of the potential curves for the low-lying electronic states. Computed potentials were approximated then by a Morse potential. Then the one-dimensional Schrödinger equations was solved using the Level code (version 8.2) [4] to find the vibration-rotational levels of the electronic states. The internal partition function was computed using our own code "Partition Function". Subsequent calculations of the thermodynamic functions for Ar_2^+ and Ar_2 were performed according to the techniques described in the reference book [5].

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Physically based mathematical model as an ordinary equation of state

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Multi-constant and low-parametrical equations of state (EOS) (including 10–15 parameters) alternate as the trend of research. The preference given to the EOS of the first type can be considered as the pursuit of mathematical precision. If the preference is given to the second ones, it does not mean their physical justification because parameters are fitting. Therefore, assuming that the parameters of EOS must have a physical sense, we investigate the equations we hope to be able solving this problem: with a small number of parameters (2–5). The purpose of the work is obtaining a simple EOS having a compromise between physical clarity and mathematical precision. These attempts result in EOS of van der Waals type and in statement: they are weakly associated with micro-level. We have shown that this may be due to an incorrect reading and interpreting information contained in the original EOS of both types resulting later in a number of cognitive problems. We use EOS based on two simplest molecular models: hard-spheres (EOS of vdW type, independent, binomial; two first parameters have sense) and point centers (EOS of one-parametrical family, trinomial, two configuration contributions, three parameters having sense). Their solution requires giving up some of the accepted ideas (starting with the van der Waals model). This new approach makes it possible to obtain non-standard information. Besides, many EOS of vdW type after reformatting can be easily written in a physically reasonable model. This, on the one hand, reduces the reproaches against them, and on the other hand, gives reason to consider the low-parameter equation obtained as a result of the sought-for compromise.

Fundamental equation of state based on new representation of scaling hypothesis

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On the basis of Scofield's linear model received a new scale representation of the hypothesis in the form of:

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

structurally having the same form as the presentation of the scale hypothesis in the Migdal's phenomenological theory of the critical point. Here X_i is one of the thermodynamic functions: isochoric heat capacity C_V, coefficient of isothermal compressibility K_T or isobaric heat capacity C_p; χ_i is the critical index equal to α if $X_i = C_V$ or γ if $X_i = K_T$ and $X_i = C_p$. It is shown that in contrast to Migdal's phenomenological theory of the approach (1), you can go to the fundamental equation of state, which carries all the characteristics and laws of the thermodynamic surface of system liquid–gas in the parameters: pressure $0 \le p/p_c \le 200$; the temperature of the triple point up to $T/T_c \le 8.2$; density $0 \le \rho/\rho_c \le 3.4$. In particular, under the proposed representation (1) is provided with accounting of asymmetry of real liquid with respect to the critical isochors in accordance with the requirements of modern physics of critical phenomena on the phase equilibrium line, the critical isotherm and critical isobar. Also provided qualitatively and quantitatively correct description of the metastable region and the transfer of border stability of the homogeneous state of a substance in accordance with the requirement. The proposed fundamental equation tested at the example of the description of the thermodynamic properties of argon, ammonia, carbon dioxide, R32.

Analysis of phase equilibrium line based on scaling hypothesis and the Gibbs–Duhem equation and Clausius–Clapeyron equation

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On the basis of the Gibbs–Duhem equation and scaling theory of the critical point is shown in terms of the thermodynamic model, the average diameter models of Yang-Yang and Wegner, describing the saturation line in the critical region, are equal. A comparison of these models on the basis of a mutually agreed system of equations, which includes the elastic line $p_s = p_s(T)$, steam branch line $\rho^- = \rho^-(T)$ and the equation for saturated liquid density $\rho^+ = \rho^+(T)$. At the same time to build a steam branch line saturation equation used Clausius–Clapeyron equation that after the introduction of heat r^*, heat of vaporization r associated with dependence $r^* = r(1 - \rho^-/\rho^+)$ is transformed into:

$$\rho^-(T) = \frac{T}{r^*}\frac{\mathrm{d}p_s(T)}{\mathrm{d}T}. \quad (1)$$

Heat r^* can be measured directly by the evaporation method [1]. It is shown that if the heat r^* is described by the relation

$$r^* = r_c\left(1 + a_1\tau^{\beta} + a_2\tau^{2\beta} + a_3\tau^{\beta+\Delta} + a_4\tau^{1-\alpha} + o\left(\tau^{1-\alpha}\right)\right), \quad (2)$$

equation (1) satisfies the mean diameter of the Wegner's model only if $a_2 = a_1^2$. Here $\tau = 1 - T/T_c$; α, β and Δ are the critical indices. If the inequality $a_2 \neq a_1^2$ equation $\rho^- = \rho^-(T)$, calculated on the basis of (1), always satisfies Yang-Yang's model.

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Joint analysis of Migdal's phenomenological theory of critical point and Benedek's hypotheses

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In [1], based on Migdal's phenomenological theory of the critical point and Benedek's hypothesis constructed nonparametric equation of state (NES) scaling type, satisfying all the requirements of a scale theory. Thus the scaling function of chemical potential has the form:

$$h\left(x\right)=A\left[\left(x+x_1\right)^{\gamma}-\left(x_1-x_0\right)^{n\beta}\left(x+x_1\right)^{\gamma-n\beta}\right]. \qquad (1)$$

In this paper we investigated different variants of NES, developed on the basis of function (1). Firstly, the variant in which $\gamma-n\beta=0$, under Griffiths conditions, critical index of critical isotherm δ is an integer $\delta\in\{3,4,5,6\}$. In this particular case, the scaling function (1) in its structure coincides with $h\left(x\right)$ Bezverkhii–Martynet–Matizen. It is shown that the function (1) satisfy Benedek's hypothesis only if the following inequality $\gamma-n\beta\neq 0$. On the basis of equation (1) calculated scaling functions of the isochoric specific heat $f\left(x\right)$, the coefficient of isothermal compressibility $f_z\left(x\right)$. A comparative analysis of the functions $h\left(x\right)$, $f\left(x\right)$, $f_z\left(x\right)$ with the respective scale functions of Scofield's linear model (LM) and Litster–Ho cubic model. As a result, it developed nonparametric scaling equation, which was tested by the example of the construction of scale equation of argon with different sets of critical exponents. It is shown that the stage of scaling equations can be expanded by using the dependence for determining the scaling function $h\left(x\right)$:

$$\Delta\mu C_V^{(\gamma+\beta)/\alpha}=\varphi_1 m+\varphi_3 m^3,\quad m=\Delta\rho C_V^{\beta/\alpha}. \qquad (2)$$

Equation (2) is calculated based on LM.

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Development of combined scaling models for liquid and gas densities at the saturation line: structures and numerical data for SF_6

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Scaling models are investigated in the form of $F(t, D, C)$ that is connected with one of thermodynamic properties $F =$ (the liquid density (ρ_l), the gas density (ρ_g), the order parameter (f_s), the mean diameter (f_d), etc.) related to the coexistence curve. This model includes critical characteristics $D =$ (the exponents, α, β, ...), a relative temperature $t = (T_c - T)/T_c$ and coefficients C. It follows to the scaling theory of critical phenomena. We have developed one more model to express f_d. It is named as a combined scaling model and includes a component with an exponent 2β, a component with an exponent $1 - \alpha$ and regular components. This model structure is estimated due to recommendations [2] and [3]. Similar combined models are elaborated to express the properties, $F = (\rho_\mathrm{l}, \rho_\mathrm{g}, f_s)$. A non-linear statistical procedure is developed to determine critical parameters (T_c, ρ_c), characteristics D and coefficients C of these combined models. We have used experimental $(\rho_\mathrm{g}, \rho_\mathrm{l}, T)$ data for the sulphur hexafluoride [3] in the procedure. The combined scaling models of liquid and gas densities are valid at $t = 0$–0.3. They are compared with some equations including a model of Anisimov *et al* (2006), a model of Fisher *et al* (2003) and a model of Wagner [3].

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Extrapolation of IAPWS-IF97 data: liquid and gas densities at the saturation line in the critical region of H_2O

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Some literature sources are analyzed in this report. They contain tabulated data on liquid (ρ_l) and gas (ρ_g) densities at the saturation line of H_2O. Among the sources there are works of Alexandrov *et al* (1980), Anisimov *et al* (1990) and [1]. A scaling model of Anisimov *et al* (1990) is valid in the critical region at $t = 0.002$–0.012 and based on old $(\rho_\mathrm{g}, \rho_\mathrm{l}, T)$ data, here $t = (T_c - T)/T_c$ is a reduced temperature. It is an interesting task to elaborate a scaling model that can represent IAPWS-IF97 data [1] in the critical region. We have involved a $F(t, D, C)$ model that is connected with one of thermodynamic properties, $F = (\rho_\mathrm{l}, \rho_\mathrm{g},$ the order parameter (f_s), the mean diameter $(f_d))$. This model includes critical characteristics, $D = (t,$ the exponents, α, β, coefficients, $C)$, and follows to the scaling theory of critical phenomena. It consists of singular and regular components. The model structure is estimated due to recommendations [2] and [3]. We have made numerical estimates of $F(t, D, C)$ parameters with an usage of tabulated (ρ_g, ρ_l, T) data on the coexistence curve of H_2O [1]. Applied $(\rho_\mathrm{g},\ \rho_\mathrm{l},\ f_s,\ f_d,\ T)$ results are got in the region $t = 0.00001$–0.1. Calculated results are compared with literature data on the properties.

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The online database for thermodynamic properties of individual substances IVTANTHERMO-Online

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Thermodynamic databases play essential role in a wide range of applications such as rocket engine engineering, nuclear power, chemical technology, metallurgy, etc. One of the most known is the IVTANTHERMO database [1] based on the reference book [2]. At present it contains properties of more than 3400 substances, formed by 96 chemical elements. A new database architecture is proposed for IVTANTHERMO that enables to obtain and update information via a modern web interface called "IVTANTHERMO-Online", to keep multiple versions of each block of data, to store additional information for users and experts (such as comments, bibliography, experimental data, molecular structure, etc.), to present data in multiple forms, to attach calculation services and link with other databases.

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Effect of overpressure in dual porous media with brittle skeleton

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If pore pressure in a reservoir is greater than the hydrostatic one, it is refereed to as overpressure. It is formed by kerogen decomposition. Overpressure can lead to the development of secondary fractures in ultra low permeable reservoirs (oil shale). This phenomenon, called natural hydraulic fracturing, is well known [1, 2]. Fracturing is the result of high in situ stresses and technological operations such as drilling and production. The concept of dual porosity is a common way for simulation of oil and gas shale production [3]. The fractured porous media is considered as the superposition of two permeable continua with mass exchange. The first media is an ultra low permeable matrix. The second is a highly permeable continuum which porosity is much lower than that of the first continuum. The most volume of oil is stored in the matrix. In this work a new generalization of dual porosity model is proposed. Damage mechanics [4] is applied for simulation of natural hydraulic fracturing in low permeability matrix. The process of the secondary microcracks development affects the matrix porosity and enhances the mass exchange between the continua. The influence of overpressure on oil production is numerically studied for a long horizontal fracture. It is shown that natural hydraulic fracturing can occur when the pore pressure in the permeable continuum near the wellbore is depleted.

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Using of capillary measurements for the filtration law restoration in the low-permeability medium

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Problem of determining the filtration law for low-permeability medium from petrophysical and well testing data was considered. It was defined that the deviation from the linear filtration law was caused by the interaction between skeleton and fluid [1]. As a result, a structure occurs at the walls of pore channel, which does not take a part in filtration [2]. The presence of boundary layer reduces effective radius of pore channel [3]. Dependence of this radius from the medium permeability and starting pressure gradient was proposed. It was found that there are some characteristic values of pore channel radius, where the motion follows fundamentally different laws. Set of methods that allow to define law of fluid motion in pore channels by means of direct and indirect measurements was considered. Main problems arising from the use of the proposed methods and ways to solve them were defined. Obtained results can be used for correct prediction of pressure field in nonlinear filtration, as well as in wells investigation in the unsteady inflow.

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4. Physics of Low Temperature Plasma

Brightness temperature and specific conductivity of multiple shocked initially gaseous protium and deuterium up to 0.4 TPa

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Brightness temperature records at wavelength of 600, 700, 734, 805, 807, 850, 900, 972 and 1500 nm from brass assemble with sapphire window, filled by gaseous isotope of hydrogen at temperature of 78 K and pressure near 20 or 9 MPa, was registered under its multiple shock compression up to 390 GPa. Electrical resistance of the hydrogen layer was measured by three electrode constant current measuring scheme simultaneously. Process of compression was simulated by 1D and 2D hydrodynamic codes with using of wide-range semiempirical equation of state (EOS) of hydrogen and other assemble materials. Results of measurements were compared with simulation results which use two hydrogen EOS model—SESAME and model with metal–insulator transition. It was shown that hydrogen conductivity increases in small region of density in accordance with proposition of plasma phase transition existence in the investigated area of states of compressed by multiple shock hydrogen.

Molecules ionization at phase transition in warm dense hydrogen

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A new idea is introduced that ionization of molecular hydrogen H_2 takes place at the fluid–fluid phase transition in warm dense hydrogen with formation of molecular ions H_2^+ and H_3^+. A conventional ab initio molecular dynamics and quantum simulation techniques are used. Proton–proton pair correlation functions (PCF) $g(r)$ and pressure are calculated. Three new PCF treatment procedures are applied. (i) PCF varies slowly with the density in the range of distances larger than 2 Å. However, the values of the PCFs first local maxima $g(r_{\max 1})$ and first local minima $g(r_{\min 1})$ are changed in the narrow density range. To emphasize the character of $g(r)$ changes, plots of $g(r_{\max 1})/g(r_{\min 1})$ are obtained. Strongly pronounced jumps for $T = 1500$, 1000 and 700 K are clear indications of the phase transition since they take place at the same densities where small density jumps are observed. (ii) The value of $r_{\max 1}$ is equal to the interatomic distance d_{H2} in the H_2 molecule. The value of $r_{\min 1}$ is close to the interatomic distances d_{H2+} and d_{H3+} in the molecular ions H_2^+ and H_3^+. Let $g_1(r)$ and $g_2(r)$ are PCF's which are the closest to the phase transition before and after it. The function $\Delta g(r) = g_2(r) - g_1(r)$ is close to zero for $r > 2$ Å, and has a deep minimum at $r = d_{H2}$ and a strongly pronounced maximum in the range from d_{H3+} to d_{H2+}. It means that the number of H_2 molecules decreases and a number of molecular ions H_2^+ and H_3^+ appears at the phase transition. (iii) The ratio of the second maxima and minima $g(r_{\max 2})/g(r_{\min 2})$ varies smoothly with the density. The PCF's obtained can be modeled by the soft sphere PCF's for r larger than 2 Å. The phase transition can be related to the Norman–Starostin plasma phase transition prediction. However, it differs from it by inherent structural changes. The study has been funded by the Russian Academic Excellence Project "5-100".

Critical point and mechanism of phase transition in warm dense hydrogen

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The mechanism of the fluid–fluid phase transition in warm dense hydrogen is suggested and the corresponding critical point is estimated in the given work. The density functional theory is applied for the calculation of the equation of state, proton–proton pair correlation functions (PCF) $g(r)$ and conductivity in the density and temperature range, where the phase transition is suggested. The VASP plane wave code is used. The values of the PCF's first local maxima $g(r_{\max 1})$ and first local minima $g(r_{\min 1})$ are changed dramatically in the narrow density range of the expected phase transition, contrary to the ratio of the second maxima and minima $g(r_{\max 2})/g(r_{\min 2})$ which varies smoothly with the density. To emphasize the character of $g(r)$ changes, the dependence of ratio $g(r_{\max 1})/g(r_{\min 1})$ on density is considered. Jumps for $T = 2500$ and 4000 K are clear indications of the phase transition at the expected densities. The dependence of discontinuity of ratio $g(r_{\max 1})/g(r_{\min 1})$ on temperature gives us the estimation of critical temperature $T_{\rm c} \sim 4000$ K which is two times higher than the value of $T_{\rm c}$ predicted in [1]. A two-step phase transition mechanism is suggested. The first stage is related to the partial ionization of H_2 molecules with formation of the molecular ions H_2^+. The second stage is the reaction of H_2 molecules and H_2^+ ions to form H_3^+ ions. Therefore, the nature of the phase transition combines the ionization and the structure transformation. The work is supported by the Russian Science Foundation (Grant No. 14-50-00124).

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Electrical conductivity of warm dense matter: Electron jellium—new gas-plasma component

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Measurements [1] of electrical conductivity in metal vapors were carried out in wide range of densities along isotherms (for temperatures above the critical). This state called warm dense matter (WDM). Continuous transition from gas-plasma to metal conductivity at density increase is shown. Existence of conductivity minimum is noted. In [2] we calculated conductivity of metal vapors directly in a critical point. Electrical conductivity in a critical point is determined via electrons of the electron jellium, appears due to overlapping of wave functions of valence electrons at compression of atoms.The idea about possible coexistence in WDM the electron jellium, as a result of cold ionization, and free electrons, as a result of thermal ionization, is advanced. We offer the Helmholtz free energy for dense atomic metal vapors describes mixture of the atoms connected by the electron jellium and also nonideal free ions and electrons. Jellium electrons exist at negative energy, and free, thermal electrons, at positive energy and they coexist independently. Concentration of electrons of jellium is determined by various ways. Concentration of thermal electrons is determined by the Saha formula. The calculations of electrical conductivity show a satisfactory agreement with experiments [1] and describe continuous transition from gas-plasma conductivity (thermal electrons, small density) to metal conductivity (jellium electrons, high density). Calculations surely show existence of a minimum of conductivity on an isotherm and explain its existence as result of change of carrier's type: from gas-plasma thermal electrons to metallic electrons of jellium.

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Solution of the "sign problem" in pair approximation

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Over the last decades significant progress has been observed in theoretical studies of thermodynamic properties of strongly correlated fermions at non-zero temperatures, which is mainly conditioned by the application of numerical simulations. The reason for this success is the possibility of an explicit representation of the density matrix in the form of the Wiener path integrals and application of the Monte-Carlo method for further calculations. The main difficulty for path integral Monte-Carlo studies of Fermi systems results from the requirement of antisymmetrization of the density matrix as in this case all thermodynamic quantities are presented as the sum of alternating sign terms related to even and odd permutations and are equal to the small difference of two large numbers, which are the sums of positive and negative terms. The numerical calculation in this case is severely hampered. This difficulty is known in the literature as the "sign problem".

In this work to overcome this issue the new numerical version of the Wigner approach to quantum mechanics for treatment thermodynamic properties of the strongly degenerated systems of interacting fermions has been developed. The new path integral representation of the quantum Wigner function in the phase space has been developed for canonical ensemble. The new quantum Monte-Carlo method for calculations of average values of arbitrary quantum operators has been proposed. To test the developed approach calculations of the momentum distribution function of the ideal strongly degenerated system of Fermi particles has been carried out. Comparison with analytical expression for ideal fermions shows a good agreement.

Calculation of quantum momentum distributions by Monte-Carlo method

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Quantum effects may strongly disturb the momentum maxwellian distribution function and are important in studies of kinetic properties of matter at low temperatures and under extreme conditions (for example, for combustion, detonation and even warm nuclear fusion). In this case particles are strongly coupled and perturbative methods can not be applied. Therefore, for theoretical studies of these systems the ab initio approaches in phase space are required. In this work we propose quantum Monte-Carlo method for calculation of distribution functions and thermodynamical properties of strongly coupled degenerate Fermi systems based on path integral representation of Wigner function.

Calculations of distribution functions and thermodynamic values can be carried out by the usual Monte-Carlo method for density matrix in path integral representation and subsequent 3-dimensional Fourier transform. This method allows to a great extent to overcome the well known sign problem for degenerate Fermi systems of particles. The method have been tested on some simple models: single particle in one and three dimensional potential wells and degenerate many particle Fermi systems. Results are in very good agreement with available analytical expressions and independent numerical data.

The thermophysical properties of Mo plasma

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The thermophysical properties (equations of state and electronic transport coefficients) of different substances under various temperatures and densities have been studied for more than hundred years. Now we have several theoretical approaches to obtain the necessary information in the metallic plasma region (see [1] for references). But for the most of metals the information about thermophysical properties of metals in this region (at T more than 5 kK) is very limited. Moreover, the temperature can not be measured directly in the available experiments yet. Nevertheless, the available measurement data [2, 3] allows one to check the existing calculation models.
To study the properties of plasma under consideration corresponding model was developed earlier [4, 5]. It allows one to calculate the chemical composition, thermodynamical values and electronic transport coefficients. The model was applied to different substances, including noble gases, several metals and semiconductors (see references in [4, 5]). It is based on the "chemical" approach (to find the plasma composition and thermodynamical values) and the relaxation time approximation (to find the coefficients). Here our model is applied to molybdenum. Namely, we have calculated the pressure, internal energy, conductivity, thermal conductivity and thermal power at $T \geq 8$ kK and densities ≤ 2 g/cm^3 for this plasma. The obtained results are in good agreement with available results of measurements and calculations of other authors.

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Recombination and electric conductivity of ion plasmas

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Ion plasmas are formed in dense electronegative media at pulse discharges for nanoseconds time as a result of the electrons attachment. Plasma lifetimes and electric energy absorption in such systems are determining factors for the dielectric strength restoration after electrical breakdown.

Mobility, recombination and electric conductivity depend on charged particles number density and Coulomb non-ideality parameter for both electron–ion and ion plasmas. In this paper, ion recombination process peculiarities are treated in the systems where Coulomb non-ideality effects are important. Dense gases systems are considered for both low and high ion concentrations.

Corrections are estimated for the classical Langevin model at the ion recombination rate calculation in dense gases. An important influence of the ion Coulomb non-ideality on the ion recombination kinetics is shown for non-ideal ion systems. The effect decreases with the increase of background gas density. An ion recombination rate calculation method is suggested which includes the influence of both background gas density and ion Coulomb non-ideality at high ion concentrations in medium.

Ion mobility and electric conductivity of ion plasmas are calculated in the range of high values of the Coulomb non-ideality. Electric conductivity dependences on the background gas pressure and ion concentration are specified in the area of high values of the Coulomb non-ideality parameter. Electric conductivity of ion plasmas is considered for high frequencies. The result is compared with the Drude model, deviations from it are shown for the high values of the Coulomb non-ideality of ion plasmas.

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Diffusion regime of ion recombination in liquid

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Recombination in non-ideal ion plasma in a liquid at diffusion regime is considered in this work. A new effect of increase of the ion recombination rate at certain ion radii is presented. The increase in recombination rate is connected with ion diffusivity and ion pair lifetime.

Dependences of ion recombination rate on ion radius are calculated by molecular dynamics in different liquids. It is found that such dependences have sharp maximums at certain ion radii. Factors that affect recombination in liquid are considered in order to explain it. First of all recombination in liquid is usually a diffusion controlled due to high density of neutral component. The direct connection between the diffusivity and recombination rate could be established using Langevin relation

$$K = 4\pi e^2 (D_+ + D_-)/kT\varepsilon, \tag{1}$$

where D_+ and D_- are the diffusion coefficients of positive and negative ions respectively. Thus the maximums observed in recombination rate could be attributed to maximums observed in ion diffusivity [1]. It is shown that they are connected with decrease of ion cluster stability. These results are additionally refined to take into account plasma coupling.

The other factor that affects recombination is a formation of a pair of cluster ions [2]. Lifetimes of such pairs as a function of ion radius are calculated and attributed to change in recombination rate.

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Optical and transport properties in partially ionized dense plasma

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Partially ionized plasmas are governed not only by the collisions of free electrons and ions but also electron–electron collisions, the ionic microfield and additional collisions due to neutral components. The ionization energy and spectral line shapes are strongly modified by a surrounding plasma environment. Starting from a generalized linear response approach, we derive consistent expressions for the dielectric function in terms of adynamical collision frequency [1, 2]. The dc conductivity of warm dense aluminum is derived from x-ray Thomson scattering data [3]. A fit formula [4, 5] is suggested. The extension to the optical conductivity within a wide frequency range [2] and the inclusion of electron–phonon collisions are discussed. The well known Ramsauer minimum observed in the transport cross section of noble gases can be described consistently using an optical potential. For the understanding of recent reflectivity measurements in Xe, also a finite Fermi-like density profile is considered [6]. Finally, for the modification of the ionization energy, described by the electronic self-energy within the framework of a quantum statistical theory, the influence of the ionic microfield is taken into account via the structure factor. We discuss the ionization potential depression.

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The investigation of polarized reflectivity properties of shock-compressed non-ideal plasma

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The study of properties of the electronic subsystem in strongly correlated plasma remains an ongoing problem in the physics of high density energy. The analysis of the response of dense plasma to electromagnetic waves of moderate intensity can be used as a tool to investigate the validity of the physical models describing the behavior of matter under extreme conditions.

The results of new experiments on reflectivity of polarized light on non-ideal xenon plasma are presented. The investigation of polarized reflectivity properties of plasma was accomplished using laser light of wavelength $\lambda_{\text{las}} = 1064$ nm ($\nu_{\text{las}} = 2.83 \times 10^{14}$ s^{-1}). In order to measure the shock-compressed xenon plasma polarized reflectivity coefficient, the pulsed YAG system with electro-optical shutter and four-channel pulse high speed device has been used. The device allows to measure the intensity of the reflected laser beam for four azimuthal angles and was equipped with filters for selection of frequency of probing. The measurements of polarized reflectivity coefficients of explosively driven dense plasmas have been carried out at incident angles up to $\theta = 55^\circ$ simultaneously for s- and p-polarization, respectively.

During the experiments, the plasma density up to $\rho = 1.8$ g/cm^3, pressure up to $P = 9$ GPa and temperature up to $T = 30000$ K were realized. Under these conditions, the plasma is non-degenerate. The integration of Maxwell equations are based on an interpolation formula for dc conductivity, obtained from a systematic quantum statistical treatment of different limiting cases.

Aqua screening properties

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Proposed is a scenario for development of observed relaxation phenomena in the pure water. ±-ions are generated by thermal dissociation of H_2O molecules. In presence of uniform electric field $E_{\|} \neq 0$, these ions forms the accumulation layers near the free surface of the liquid.

After accumulation near the free surface of the liquid with a finite density n_s the ions can break its stability producing a pulse of ion current to the collector located above the liquid surface. The outlined process is periodically repeated. Its period contains information on the ion mobility and, which is most interesting, on dissociation (association) processes occurring in a system of charged particles placed in an external field. The cryogenic problem is a good model for dissociation in the presence of external field occurring in normal electrolytes without any external ion sources.

Bose condensation and the problem of bozonization of fermions

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The problem of creation of bosons in a system of fermions is discussed. This problem is straightforward related with mechanisms of superfluidity of He_2 and superconductivity. Till now there is no clear understanding how interaction between fermions can lead to the composite boson state [1, 2]. In the report the various opportunities for solution of this problem are discussed.

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Frequency depending permittivity of the model Coulomb system with Bose–Einstein condensate of nuclei

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The second-order singularity is found in the low-frequency region of the permittivity $\varepsilon(\omega)$ of a homogeneous and isotropic system of charged particles consisting of electrons and boson nuclei

$$\varepsilon(\omega) \mid_{\omega\to 0}\to -\frac{\omega_{\mathrm{BEC}}^2}{\omega^2}, \tag{1}$$

where

$$\omega^{\mathrm{BEC}} = \sqrt{\frac{4\pi z^2 e^2 n^{\mathrm{BEC}}}{m_{\mathrm{c}}}} \tag{2}$$

is the characteristic frequency of the Bose-condensed nuclei with the density n^{BEC} and the mass m_{c}. Above the transition temperature T_{c} the value n^{BEC} equals zero. This singularity is caused by the existence of a Bose–Einstein condensate for nuclei. The result leads to the existence of the "nuclei superconductivity", which can be experimentally verified in superfluid He_2 [1]. The results of the proposed an experiment can be considered as a direct proof of the existence of a Bose–Einstein condensate in superfluid He_2.

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Influence of the electron intrinsic magnetic moment on the transverse dielectric permittivity of a degenerate electron gas

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Using the linear response theory, the transverse dielectric permittivity $\varepsilon^{\rm tr}(q,\omega)$ of a homogeneous and isotropic system of charged particles, a common form of which is determined by the ratio

$$\varepsilon^{\rm tr}(q,\omega) = 1 - \frac{\omega_{\rm p}^2}{\omega^2} - \frac{4\pi}{\omega^2}[\varphi_{\rm d}(q,\omega) + \varphi_{\rm p}(q,\omega)], \qquad (1)$$

is considered. Here $\omega_{\rm p}$ is the plasma frequency, $\varphi_{\rm d}(q,\omega)$ and $\varphi_{\rm p}(q,\omega)$ are the correlation functions of the operators of electric currents without explicit accounting and with consistent acconting of the intrinsic magnetic moment of charged particles, respectively [1]. The relation is used in the application to the liquid metal plasma, which is characterized by weak electron–ion and moderate electron–electron interactions [2]. On this basis, in the ideal gas approximation an explicit analytical expression for the transverse permittivity of a degenerate electron plasma, which takes into account electron spin, is found. This result takes into account both the Landau diamagnetism and Pauli paramagnetism in the electron plasma. The influence of the electron intrinsic magnetic moment on the spatial and frequency dispersion of the transverse dielectric permittivity degenerate electron plasma is studied, that is crucial for determining the optical characteristics of plasma [3].

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Simulation of self-diffusion in strongly coupled plasmas by molecular dynamic method

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Our work concerns a simulation of heavy charged particles energy relaxation in electron gas. We used numerical simulation as a tool to test existing theoretical approaches to classical Coulomb system kinetics. Using molecular dynamics method we calculated dynamics of energy relaxation of protons in ultracold electron gas. We considered as neutral and non-neutral plasma when number of electrons is much greater than the number of protons. In the computer experiments we calculated the velocity autocorrelation function for charges in overcooled plasma. We have shown that boundary conditions have significant influence on simulation results. Two types of boundary conditions were considered: periodic boundary conditions and reflecting walls. The influence of number of particles in simulation cell was studied. The problem of Coulomb potential modification on small distances was also considered. The work was supported by the Russian Science Foundation, grant No. 14-19-01492.

Self-diffusion and conductivity in ultracold strongly coupled plasma: The calculation by the molecular dynamic method

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We present the result by the calculation molecular dynamic method self-diffusion and conductivity of electron and ion components ultracold plasma, including in the presence of the magnetic field. There is a comparison with available theoretical and experimental data.

New opportunities for studies of ultracold Rydberg atoms with many-photon coherent spectroscopy

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Goal of our research is preparation and study of ultracold Rydberg matter which was suggested by E A Manykin *et al* in 1980 [1]. Recently many publications are devoted to study of ensembles of ultracold highly excited atoms and strong coupling plasma of alcaly and alcaly earth elements [2]. New exotic Rydberg molecules like "butterfly molecules" were created [3]. Ability to control of excitation and position of Rydberg atoms will allow to get qubits [4].

At our setup we performed experiments for preparation of ultracold Rydberg atoms and diagnostic of energies and spectral width of quantum Rydberg states by using developed spectroscopic method. Spectral broadening due to electric and magnetic fields, or thermal atomic motion, was measured. As the next step we suggest to use pulse four-wave mixing technique for investigation of kinetics and thermodynamics in system of ultracold Rydberg atoms.
This work was supported by the Russian Science Foundation (project No. 14-50-00124).

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Width of Rydberg *nS*- and *nD*-sates for different quantum numbers *n*

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By using spectroscopic technique based on recording variation of the resonance fluorescence in magneto-optical trap (MOT) [1,2] the narrow resonances were observed on coherent two-photon transitions to Rydberg states with principal quantum number from 38 to 120. The width of nS states does not depend on quantum number n. It is defined by the temperature of atoms in the MOT and the intensities of cooling beams. Observed broadening of coherent resonance on two-photon transition $2S$–$2P$–$82D$ is attributed to simultaneous excitation of forbidden transitions to Rydberg states $82D$ with large L (from 3 to 20).
This work was supported by the Russian Science Foundation (project No. 14-50-00124).

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Dipole interatomic interactions in hot and ultracold gases

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In presentation our experimental and theoretical studies of dipole–dipole interactions between atoms will be discussed. Classical dipole–dipole interactions occur between atoms in the ground state and in the first excited state [1]. Potential for dipole interactions is $V(r) = d^2 r^{-3}$. In a resonance gas with density N the effective potential can be written as $V = d^2 N$. In hot gases ($T > 300$ K) the potential V is much less than the energy of atomic thermal motion $kT = mv_{\rm th}^2/2$. Therefore the dipole interactions induce only to the spectral broadening of atomic transitions $\Gamma = d^2 N/h$. We find that the dipole broadening in partly excited hot gases is different in dilute and dense gases [2]. In the dilute gas ($\Gamma \ll \omega v_{\rm th}/c$) Γ does not dependent on level of excitation. In the dense gas ($\Gamma \gg \omega v_{\rm th}/c$) Γ can be strongly reduced by optical excitation [2]. The study of ultracold Rydberg atoms can reveal new opportunities and effects. Such atoms have unique properties as long radiative lifetime and strong dipole interactions. (i) Low density gas of ultracold Rydberg atoms: $V \ll kT$. The interatomic interactions can induce energy shift of quantum states which results in Rydberg blockade. (ii) High density gas of ultracold Rydberg atoms: $V \geq kT$. The dipole interactions can change the motion of Rydberg atoms. Under these conditions chains and periodic structures can appear [3].

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Approach to produce antihydrogen atoms with low kinetic energy in magnetic traps

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Antihydrogen atoms are produced in Penning–Malmberg traps when antiprotons are injected into the cloud of ultracold positrons [1]. After the mixing, non-neutral plasma of antiparticles is formed and atoms are created during three-body recombination process. The main problem in the experiments is increasing the very low number of atoms formed. This is due to the low depth of the atomic trap ~ 0.5 K and the high initial energies of antiparticles, which may reach hundreds of K and more.

Our present study is concerned with finding the ways to increase the antihydrogen yield. Previously, we reported our progress in this direction: using the molecular dynamics method we were able to calculate the energy relaxation rates for antiprotons in experimental conditions. In the present work, we study the particle interaction in a wider range of densities, energies and magnetic field magnitudes. We show that some changes in experimental conditions can provide acceleration of cooling of antiprotons, which in turn can lead to the decrease of atomic temperature and the possibility of capturing more atoms. Moreover, we derived analytical expressions for the cooling rates based on our calculations, which are in qualitative agreement with the experiments results.

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Experimental setup for laser cooling and trapping of calcium atoms

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Our goal is creation and study of ultracold dense gases of Rydberg lithium and calcium atoms [1,2]. We have investigated Doppler-free resonances at atomic transition with wavelength 423 nm in high temperature cells with cold windows. The saturation resonances will be used for frequency stabilization of tunable lasers which will be applied for laser cooling and trapping of calcium atoms. The linewidth of the observed saturation resonance was about 55 MHz, with a natural width of 34 MHz [3].

Also we start assemble vacuum part of experimental setup for laser cooling and trapping of calcium atoms. As the first step the Zeeman slower for cooling calcium atoms has been developed.

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Simulation of cathode spot formation in arc discharges

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The paper is presented a self-consistent model describing the dynamics of the ignition arc and the dynamics of the formation of the cathode current spots. The model is based on a self-consistent description of the processes occurring at the electrodes and in the discharge gap. To describe the behavior of charged and excited particles used fluid approximation, self-consistent field in the plasma and the potential profile in the space charge layers are determined from the Poisson equation. Description of the processes occurring with participation of electrons is based on the solution of the Boltzmann equation. Furthermore, the system of equations includes the energy balance equation of the electrons and heavy particles. To describe the processes occurring at the cathode, formulated heat balance equation for the cathode and differential Ohm's law. At the boundary between the plasma and the cathode were considered conjugate effects: heat flux from the plasma to the cathode, bombardment by charged particles, thermal emission of electrons from the cathode, and others. On the basis of the evolutionary model we performed a series of numerical experiments to study the dynamics of arc ignition, depending on various external factors. The main result of these experiments is to demonstrate the dynamics of the ignition of the arc discharge [1], as well as the temporal evolution of the formation of the current cathode spot. This work was supported by the Russian Foundation for Basic Research (project No. 16-38-60187)

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Microcrater formation model in the cathode spot cell of a vacuum arc

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The miscocraters formed on the cathode of a vacuum arc are the result of extrusion of the molten cathode metal under the pressure of the cathode spot plasma [1, 2]. A semi-empirical hydrodynamic model based on the cellular structure of the cathode spot of a vacuum arc has been developed to describe the formation of a microcrater on the cathode and the initial axisymmetric stage of the formation of liquidmetal jets [3]. In the context of a 2D axisymmetric problem statement of charge, heat, and mass transfer in a cathode, the formation of a crater on a copper cathode has been simulated for a constant current carried by an individual cathode spot cell. It has been shown that for the cell current ranging between 1.6 and 7 A and the time of current flow through a cell ranging between 15 and 60 ns, the crater diameter is 3–7 μm. In these cases, the current density at the center of a cathode spot cell is 10^{12} A/m^2, and the average current density in a cell, determined using the crater diameter, is 10^{11} A/m^2. The obtained results are in agreement with experimental data on the crater size, cathode spot lifetime, and cathode spot current density at near-threshold arc currents [4, 5].

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Formation of liquid-metal jets in a vacuum arc cathode spot: Analogy with drop impact on a solid surface

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In reference [1] it was pointed out that the behavior of a liquid metal extruded from craters produced on a cathode during vacuum arc burning is analogous to the behavior of liquid during the fall of drops on a solid flat surface. In both cases, the main parameters describing the behavior of the system are the size of the region initially filled with liquid and its characteristic velocity. However, while the characteristic times for hydrodynamic processes in the cathode spot are a few or dozens of nanoseconds and the characteristic scale is a few microns [2], which complicates their *in situ* observation, the typical time, and spatial scales in the problem of collisions of drops with obstacles are as a rule milliseconds and millimeters, respectively. As a result, numerous experimental data [3] are available on the behavior of liquid drops and, in particular, on the conditions of liquid splashing in the latter case. In the present work we demonstrate that the main parameters describing fluid motion (the Weber, Reynolds, and Ohnesorge numbers) fall into the same intervals for both mentioned problems. Then, according to hydrodynamic similarity principles (processes in geometrically similar systems will proceed similarly when the numbers We, Re, and Oh coincide), we can apply the known splashing criteria [3] to analyze conditions for liquid-metal jets formation during vacuum arc burning. The work was supported by the Russian Foundation for Basic Research (projects No. 16-08-00228 and 17-08-00430).

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A model of the retrograde motion of the cathode spot of a vacuum arc in an external tangential magnetic field

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The physical processes that accompany the retrograde motion of the cathode spot of a vacuum arc in an external tangential magnetic field are considered based on the principle of maximum magnetic field. It is shown that the magnetic field causes an asymmetry in the plasma density distribution at the boundary of the plasma jet ejected from the cathode spot, but it has no effect on the physical processes that occur immediately in the spot. Cathode spot extinction is accompanied by ejection of plasma toward the site where the total magnetic field (the external field plus the self-magnetic field of the cathode plasma jet) is a maximum. At this site, a new spot is born. The velocity of the directed motion of a cathode spot in an external magnetic field increases with current mainly due to an increase in geometric size of the spot operation area. This velocity increases linearly with magnetic field until reaching a saturation value. The maximum velocity of motion of a cathode spot corresponds to the velocity of its random motion at a given arc current. This work was supported in part of by the Russian Foundation for Basic Research under grant No. 16-58-50015, and by the Russian Academy of Sciences under the basic research programm No. I.9P.

Effect of the nanostructured layer thickness on the dynamics of cathode spots on tungsten

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Experimental data on the effect of the thickness of a nanostructured layer present on the surface of a tungsten cathode on its arcing properties have been analyzed. It has been found that the key parameters that are responsible for the arc initiation are the electrode potential, which must be no less than 50 V, and a threshold pulsed power of the external action on the cathode. For the arc operation to be self-sustained, its current should be above a threshold value depending on the properties of the nanostructured surface. To model the grouping feature of arc spot cells, an attractive force was introduced into a random walk model based on the Monte-Carlo method. It has been demonstrated that spot cells are entangled, forming a group, and move together when the attractive force between them is strong enough. A decrease in this force and an increase in the directionality of the cells of a cathode spot as it shifts on a lower thickness of nanostructure layer result in an increase in the velocity of motion of the spot and in a decrease in the width of its trail left on the surface. The study was supported in part by the Russian Foundation for Basic Research (project No. 16-58-50015).

Explosive electron emission, plasma parameters, evaluation from the liquid-metal jet tearing model

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A simple complete model has been proposed for the explosive emission pulse of the cathode spot cell that involves both—the ignition and the decay of the explosive plasma. The ignition is due to the hydrodynamic tearing of the liquid-metal jet, propagating into the plasma generated by the preceding explosive cell. The decay is due to the plasma expansion and the density decrease down to the initial. The explosion per se is treated as the transition of the jet material over the critical state. The average parameters of the plasma have been evaluated. In particular, the plasma basic parameters—the density and temperature are about 10^{20} cm^{-3} and 1 eV respectively. The average ratio of the pressure to the current density has been evaluated $p/j \approx n_0 T_{\rm cr}/j_{\rm max}$. This ratio gives a specific plasma acceleration force, and the obtained value that is about tens of gcm/Cs agrees with the measured recoil force and with the product of measured ion velocity and erosion. The average ohmic electric field has been found to be several tens of kV/cm. This field is responsible for the current transfer through the explosive plasma and, hence, the cathode potential fall formation. For the known cathode potential fall, the corresponding specific plasma size is several micrometers. In addition, the total current flowing through an exploding liquid-metal jet has been estimated to be some amperes. General estimate of the plasma–to–magnetic pressure ratio, for a current-carrying plasma column has been derived that indicates that the column compression by a magnetic ($\beta < 1$) takes place only for large-scale low-density ($nR^2 > 10^{14}$ cm^{-1}), such that occurs far from explosive cells. Work supported by grants No. 15-38-20617 and 16-08-01397 from the Russian Foundation for Basic Research.

Calculation of parameters of avalanche of runaway electrons

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With the help of the numerical model are investigated regularities avalanche of runaway electrons in air at atmospheric pressure. The results of numerical calculations show that in addition to characteristic time and length by an exponential increase of the avalanche of runaway electrons can be characterized by other parameters such as the velocity of propagation of avalanches and the average kinetic energy of runaway electrons.

Large-scale instabilities developed on the surface of aluminum conductors at strong magnetic fields

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The experimental results on electrical explosion of aluminum cylindrical conductors with a diameter of 2 mm at the magnetic field up to 400 T is presented. The experiments were carried out on the MIG high-current generator at a current level up to 2.5 MA with a current rise time of 100 ns.

Study of delay plasma formation on the surface of double-layer conductors in strong magnetic fields

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The main purpose in the design of the load assembly in high-current generators is to increase the time preceding the plasma generation on the electrode surface and to decrease the velocity of its expansion. In this paper the skin explosion of thick homogeneous and double-layer cylindrical conductors were studied at the threshold values of the magnetic field 200–400 T. Double-layer conductors were prepared by following technique. The outer layer of low conductivity and a thickness of 20–80 μm or a dielectric layer thickness of 10 μm was deposited on a copper or duralumin conductor by a vacuum arc method. The experiments were carried out on the MIG high-current generator at a current level of up to 2.5 MA with a current rise time of 100 ns. It is shown that delay process of plasma formation higher 200 ns takes place at the use of double-layer structure conductor with a low conductivity outer layer compared with the homogeneous copper or duralumin conductor. Calculations have shown that a delay of plasma formation can occur due to redistribution of the current density over the cross-section and reduce of the Joule heat on the surface of the double-layer conductor.

Openable coil for magnetic pulse industrial applications

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In industrial applications of pulsed magnetic processes, opening of the solenoids can be required, for reasons such as extracting finished, long, or closed work-piece, getting into place or around protrusions, etc. Traditional methods for constructing open-able coils use various types of contacts to provide a way for the working current to flow from one part of the coil to another. This method, however, is not suitable for pulse-power current magnitudes, which reach hundreds of kilo amperes and have very high rise rates. In conditions such as these, currents will not flow through the whole contact area, but rather through its linear circumference. A more effective way is to have Inductive connection between coil's parts. One-turn and multi-turn systems based on inductive connection from fixed power source to movable parts of coil have been developed, designed and produced. Experimental samples of these coils were tested at different current and frequency regimes, and the main factors governing the coil's efficiency in one-turn and multi-turn systems were noted. Efficiencies of 70–80% that of the baseline conventional (solid non-opening) coils of the same type and dimensions were achieved, leading to the design of pre-industrial technology demonstrators. These beta-systems were used for industrial tests, with good result.

Investigation of experimental models of microsecond duration powerful generators of current pulses based on capacitive storage and explosive magnetic generators

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Experimental models of microsecond duration powerful generators of current pulses on the basis of explosive magnetic generators and voltage impulse generator have been developed for the electromagnetic pulse effects on energy facilities to verify their stability. Exacerbation of voltage pulse carried out through the use of electroexplosive current interrupter made of copper wires with diameters of 80 and 120 μm. Experimental results of these models investigation are represented. Voltage fronts to 100 ns and the electric field strength of 800 kV per meter were registered.

Investigation of implosion dynamic of aluminum wire array on polymer cylinder at the Angara 5-1 facility

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The implosion of aluminum wire array on polymer cylinder was studied on the installation Angara-5-1 (3.5 MA, 100 ns). The array consist of 8–30 Al wires with a diameter of 15 μm. The cylinder were made from agar–agar foam of 0.01–0.02 g/cm^3 and a diameter of 1–1.8 mm or from deuterated polyethylene with density of 0.07 g/cm^3 and a diameter of 1–1.2 mm. Z-pinch plasma parameters were determined using the diagnostic set of the Angara-5-1, which includes 10-frame camera (the exposure frame 2 ns) in vacuum-uv spectral region, an optical streak-camera, time-integrated 3-channel x-ray pinhole camera with different filters, vacuum photoemission detectors, crystal spectrograph, neutron scintillation detectors. The total neutron yield was measured by activation detectors. It was found that a compact pinch with a diameter of ≈ 0.5 mm if formed and accompanied by the pulse of soft x-ray radiation. The development of magneto-hydrodynamic instabilities leads to the appearance of hot spots with a size of 200–300 μm in the range of energies $E > 600$ eV and generation of neutrons. Typical value of temperature at the pinch was 0.5–0.7 keV. The mean energy of neutrons were 2.7 ± 0.2 MeV. The maximum neutron yield was equal of 2.6×10^{10}.

Study of the hard x-ray emission specific features of plasma focus discharge with 1.5 MA pinch current

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This work describes the plasma focus (PF) device based on the capacity energy storage. It has storage energy up to 150 kJ that provides the discharge current amplitude 2 MA in the PF chamber. The device uses two types of electric switches: pseudospark switch TDI1-50k/45 and vacuum switch CVS-47 for energy transmission from capacitor storage to the load. Pseudospark commutators provide monotonous current rise on the initial stage of the discharge dynamic that forms homogeneous plasma-current sheath. After this vacuum switch sections connects and provides the discharge current rise to the maximum value. This work presents the experimental results and MicroCap simulation of PF device operation with two types of commutators.

For hard x-ray (HXR) emission studying PF chamber has been elaborated. It has a special anode inset and diagnostic windows on the cathode for HXR radiation output. PF chamber as a part of PF device was investigated with different x-ray targets on the anode. PF chamber with 1.5 MA discharge current generates HXR pulse with mean duration 16 ns and energy spectrum from 10 to 200 keV that provides the absorbed dose in samples about 1 Sv.

Electric characteristic measurements in high-current high-pressure discharge with current amplitude of 590–1200 kA by magnetic probe

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Soft x-ray radiation (SRX) oscillation were registered for discharge with current amplitude of 1200 kA at initial hydrogen pressure of 5 MPa. Near current maximum the fluctuations of SRX from the channel have been registered. Estimations of such oscillations were made. Speed of current channel contraction, channel radius and its oscillation amplitude for current amplitude of 1200 kA were measured by magnetic probe with extrapolation for currents of 590 and 900 kA.

The electric field strength in discharge channel and near electrode voltage drops was determined by comparison of channel radius oscillations with synchronous voltage changing. Also this method was used for oscillation amplitude estimation at current of 1200 kA. Satisfactory agreement for the estimations was received. Oscillation amplitudes are needed for calculation of X-ray intensity modulation. Channel plasma parameters were determined for maximal contraction moment.

The work is partially supported by Russian Foundation for Basic Research (grants No. 15-08-04219-a and 16-08-00767-a).

Investigation of vortex flows and electrical discharges forming under the action of external magnetic field in the system with liquid metal

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Electrovortex flows are the part of many technological processes. For example they take place in the working areas of such industrial facilities as: electro-arc furnaces and reactors in metallurgy and waste recycling, electroslag remelting and welding apparatus. Basically the described systems look like the following one: working area is the container filled with electro-conducting material, electric current passes through the melt from the rod electrode towards the volume one, there are systems with the electric arc between the rod electrode and the melt and without the electric arc, the electric current interacts with its own magnetic field and as a result under the action of electromotive body force the electrovortex flow appears in the system. In the presence of external magnetic field there is also azimuthal rotation of the melt and additional secondary vortex structures appear. The work will consider the different kinds of vortexes forming under the electromagnetic action and some attendant phenomenon like appearance of electrical discharges. We investigate the system experimentally and numerically. Experimental setup consists of following elements: a copper hemispherical container filled with indium–gallium–tin eutectic alloy that serves as a volume electrode, a copper or steel rod electrode with hemispherical tip that is immersed into the alloy, a coil used to create the external magnetic field in the system. Numerical investigations are based on magneto-hydro-dynamical model in electro-dynamical approach. The work is supported by grant No,i15-38-70016 from the Russian Foundation for Basic Research.

Frequency-dependent transition of surface dielectric-barrier discharge from homogeneous to constricted mode and its effect on biological target

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The increase in supplied ac voltage frequency at saving the voltage across an electrode assembly leads to transition of the surface dielectric-barrier discharge (SDBD) from uniform type to contracted one. Currently, the significance of the transition of the glow to the filamentary discharge at the treatments of biological objects is still unclear. In particular, plant samples which are in a state of physiological dormancy and, consequently, are highly protected from negative impacts, are especially attractive to study.
The experimental investigation of the effect of SDBD plasma on the early in dark germination of high-quality soft winter wheat seeds has been presented. SDBD was ignited by the sinusoidal voltage of 3.5 kV RMS at frequency range from 0.05 to 66 kHz. In all the experiments the seeds were exposed by plasma for 1 minute at a distance of 10 mm from the surface of the dielectric barrier. The treated seeds were germinated on moistened filter paper in the thermostatically controlled environment in the dark. Morphological test on lengths of sprouts and separate roots and a seed germination test were carried out on the third day of germination. Transition to constrict form of SDBD is not caused critical damages in seed. However, maximum stimulation response of morphological characteristics obtained below transition frequency.

Mass analysis of the gas composition after the electrical explosion of copper spirals with a dielectric coating

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The experiments were carried out in air atmosphere, we used four spirals, which were mounted on a textolite basis, and the neighboring spiral had opposite direction of windings (left and right). As a result, the parallel electrical connection of spirals formed of a toroidal magnetic field. Each spiral had 10 turns of copper wire with a diameter of 0.75 mm, the size of the toroidal structure was 32 mm (small radius of the torus is 4 mm, the large radius 12 mm). Wire was wrapped in capacitor paper with a thickness of 0.05 mm to prevent inter-turn short circuit. In the experiments on spiral fed a current pulse with an amplitude of about 40 kA, pulse duration was about 0.3 milliseconds. In the electric explosion of spirals was formed by the plasma clot with a life time of about 60 milliseconds. Before and after electric explosion of spirals we took samples of the gases and their mass analysis was performed using the monopole mass analyzer. The sample was introduced into the ion source in the gaseous state, and then made its ionization by electron impact with an electron energy of about 80 eV. The initial energy of injected ions is 4 eV. Spectrum scan was carried out in the range of 10 to 100 a.m.u. In the spectrum of the sample after the electric explosion of spirals were discovered new components with masses of 20, 29, and 81 a.m.u.

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Antineutrino oscillations and energy distributions of fast particles in fission plasma

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Theory and numerical simulations of degradation spectra (DS) of electrons in fission plasma in the nuclear reaction of helium-3 isotope (^{3}He + n $\rightarrow$ p + T + 0.76 MeV) are presented. Radioactive decay, nuclear fission are resulting fast particle, among them β-electrons and their immanent satellite antineutrino. Theory is based on the power spectra of degradation charged particles as the spectra with fluxes in energy space. Numerical calculations of the electron energy distribution function have been performed for He—fission fragments constituted of fission fragments under influence of high energy electron source, with detailed elementary electron collision processes with molecules and atoms being taken into consideration. The energy expenses of electrons into ionization, dissociation and excitation of various levels have been obtained so that to determine the rates of electron collision processes. The dependence of the electron energy expenses into various inelastic electronic processes upon the energy of primary electron source has been revealed. The results are presented for the rates of numerous elementary processes of electron interaction with basic ionospheric components to be suitably determined. Antineutrino appears simultaneously with the secondary electrons, and they have been measured in fusion products. The comparison of DS secondary electrons compared with the spectrum of antineutrino and conclusion about the consistency of calculated DS and antineutrino spectrum followed.

On DD and p + ^{11}B "burning" at inertial electrostatic confinement scheme in vacuum discharge

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The yield of DD neutrons in a compact nanosecond vacuum discharge (NVD) of low energy with deuterated Pd anode have been observed [1]. Further, detailed PIC simulation by the electrodynamics code KARAT have recognized that experiment with NVD have represented the realization of rather well-known scheme of inertial electrostatic confinement (IEC) [1]. Here we report on the recent progress at the studying of nuclear burning in IEC scheme based on NVD. Three directions are developing. First one is PIC-simulation of neutron-free reaction of proton–boron nuclear burning. This reaction is accompanied with the yield of three alpha particles ($p + {}^{11}B \rightarrow \alpha + {}^{8}Be^{*} \rightarrow 3\alpha$) and has the great fundamental and applied interest [2]. Second one is the relations of similarity are obtained for neutron yield and parameters of the plasma formed by the convergence of oscillating flow of ions to the axis of cylindrical system with IEC. The conditions of attainment of intense neutron generation and positive energy output (analogue of Lawson criterion [3]) are discussed. Third one, the results of a recent series of DD fusion experiments on the anew created experimental stand NVD-2 combined with x-ray and neutron yield diagnostics are presented and discussed. This work was supported by the grant No. 14-50-00124 of the Russian Science Foundation.

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Ionization–emission processes in a near-electrode plasma of high voltage air spark

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Mechanisms of plasma and emissions generating, etc. may be associated with a rapid ($\sim$ 1 ns or less) localized (micron-scale characteristic dimensions) processes that occur at the interface of the electrode material and the gas gap. As the near-electrode process, scaled-up to the extent of inter-electrode can be regarded as the mode of electrical breakdown in the switched long atmosphere gaps, formed by an exploding wire [1, 2]. Comparison of the temperature in the atmospheric discharge channel (up to $\sim$ 3 eV, using relative intensity of lines) with the spectral characteristics in the case of an additional electrode-erosion plasma, reveals the spatial features of the breakdown processes.

The conditions of plasma formation and emission processes simulated by different wire loads (Cu, Ni, NiCr, CuMnNi of 50–130 mm in diameter) in the electrode gap length of 350–700 mm.

The results of the spectral measurements (integrated and time-based) of atmospheric discharge at optical wavelengths are presented. It noted the formation of structures of different scales: the strata in the core of an electrically exploded wire, helical shaped relaxation stage of discharge channel with the lead of hundreds of times greater than the diameter of the channel. The resulting parameters are compared with the properties of materials and wire current–voltage characteristics of the discharge.

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Active Brownian motion and structures of grains in strongly coupled dusty plasma

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We study Brownian motion of metal coated grains, suspended in gas discharge, under laser irradiation. The motion is caused by photophoresis: i.e., absorption of a laser at the metal-coated surface of the particle creates radiometric force which in turn drives the particle. The grains are injected into the rf gas discharge and gain sufficiently high electrical charge ($\sim 10^2$–10^5 of electron charge) under the flows of plasma particles or in the emission processes. These charged grains effectively interact between each other as well as with external electrical field. The action of external forces and forces of interparticle interaction combined with dissipative mechanisms in these systems can lead to the self-organization of the system, resulting in formation of quasi-stationary crystal or liquid-like structures. We observed experimentally the active Brownian motion (irregular or directed) caused by radiometric force at different Coulomb coupling of the charged grains.

Dusty plasmas in the lunar exosphere: Effects of meteoroids

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Effects of meteoroid impacts from the viewpoint of formation of dusty plasma system in the lunar exosphere are considered. The main attention is paid to large altitudes over the lunar surface including the range of the altitudes between 30 and 110 km where the measurements of dust were performed within the NASA LADEE mission. We find the number densities of dust at these altitudes. The agreement between theory and experimental (LADEE) data is shown. This work was carried out as part of the Russian Academy of Sciences Presidium program No. 7 and was supported by the Russian Foundation for Basic Research (project No. 15-02-05627).

Preliminary modeling of dusty plasma environment near the Moon surface

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One of the complicating factors of the future robotic and human lunar landing missions is the influence of the dust. The absence of

an atmosphere on the Moon's surface is leading to the compaction and sintering of the dust particles found on the Moon surface. Properties of regolith as well as near-surface lunar exosphere depend on many factors, including the solar activity, lunar local time, position of the Moon relative to the Earth's magnetotail. The upper insulating regolith layer is electrically charging by photoelectron emission due to solar uv radiation and solar wind particles. Positive charge is created on the lunar illuminated side, while its night side is negatively charged. Charge distribution and thus surface potential, depend on the lunar local time, latitude and the electrical properties of the regolith (the presence of water in the upper layer of the regolith, for example, might change the regolith electric conductivity). Understanding of mechanisms of the dust electric charging, dust levitation is essential for interpretation of measurements of two instruments: Dust Impact sensor and Langmuir Probe included in the forthcoming Luna-Glob lander mission that is under development now according to the Russian space program.

Modification and destruction of the Coulomb cluster in a cusp magnetic trap at gradual increase its charge

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Experiments "Coulomb crystals" on the International Space Station using a cusp magnetic trap for diamagnetic (graphite) particles go

on. In the latter experiment a cluster has been formed of 30000 uncharged graphite particles of size 300 μm. Their charging was carried out gradually increasing the central electrode potential up to 150 V in four steps by 37.5 V each with an interval of about 15 s. Increasing the potential initially resulted to hardly noticeable (at the first step) and then to more intensive particle scattering from the cluster surface mainly in the form of filamentary complexes. But at 112.5 V, we see the escape of some individual particles (with velocities 1–4.5 cm/s). In 3 steps (45 s) the cluster lost about half of the particles. After increasing the potential up to 150 V the cluster is destroyed completely during 8 s. Estimates of the particle charge on the cluster surface have been performed by 2 ways, using depending on the cluster capacity and using their velocities observed. It is shown that the adhesion forces between particles play an important role in the balance of interparticle forces. The work was supported by the Russian Science Foundation, grant No. 14-50-00124.

Influence of dust particles on the neon spectral line intensities at the space apparatus "Plasma Kristall–4"

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The "Plasma Kristall–4" (PK-4) is a new joint Russia–Europe space experiment on board of the International Space Station operated since 2015 [1]. The aim of the experiment is the investigation of structural and dynamic properties of dust plasma in the combined dc–rf discharge under the microgravity conditions. In this work, we perform an investigation of the influence of dust particles on

the neon spectral line intensities at the uniform positive column of the dc discharge at the space apparatus PK-4 during commissioning the experiments in June, 2015. The plasma emissive spectrum was registered by Ocean Optics USB2000+ mini-spectrometer within the spectral range of 350–1100 nm with the spectral resolution of 1.5 nm. The plasma emission of the positive column was recorded with and without the dust cloud. There were obtained spectral intensity ratios of neon line intensities from the center of the dust cloud and its edge to the spectral line intensities in the undisturbed region of the uniform positive column. The obtained experimental results are discussed. The operation of the space experiment PK-4 is supported by the Russian State Corporation ROSCOSMOS and the European Space Agency.

[1] Pustylnik M *et al* 2016 *Rev. Sci. Instrum.* **87**

Phenomena in complex (dusty) plasma studied under microgravity conditions

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Complex (dusty) plasmas are composed of weakly ionised gas and charged microparticles and represent the plasma state of soft matter [1]. Due to the "heavy" component, microparticles, and the low density of the surrounding medium, the rarefied gas and plasma, it is necessary to perform experiments under microgravity conditions to cover a broad range of experimental parameters which are not available on ground. The investigations have been performed onboard the International Space Station (ISS) with the help of the PK-3 Plus laboratory. This laboratory was mainly built to investigate the crystalline state of complex plasma, the so-called plasma

crystal, its phase transitions and processes in multi-particle mixtures. Due to the manipulation of the interaction potential between the microparticles it is possible to initiate a phase transition from isotropic plasma into electrorheological plasma. The crystal–liquid phase transition was obtained in large 3D isotropic dusty plasma system. The compression of the dust particle subsystem can result in melting of the plasma crystals. Different research achievements of PK-3 Plus on the ISS will be discussed as well.

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The impact of the laser intensity on the mean-square displacement of dust particles in rf discharge

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The investigation of transport properties of the Brownian systems is relevant for various scientific and technological fields. The information of the mean-square displacement of particles within a wide time scale allows to make conclusions about the character of their interaction [1, 2], obtain various properties of particles and their surroundings [2], and, moreover, consider the degree of activity of particles [3]. This work is aimed at the experimental study of the mean-square displacement of particles in the monolayer dusty plasma structure for different values of the kinetic energy of the dust particles in it. The experiments were held in the gas-discharge vacuum chamber. The plastic melamine formaldehyde particles, covered with copper (the layer of 9.95 μm thickness) were injected in the discharge chamber. The argon was used as a buffer gas. The

dusty plasma system was illuminated by the laser radiation of various intensity that caused the change of the kinetic energy of grains. The obtained video data were processed by the special script, and as a result, the following properties of particles were obtained: coordinates, velocities, trajectories, the coupling parameter, pair correlation functions and the time dependencies of the mean-square displacements.

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[3] Golestanian R 2009 *Phys. Rev. Lett.* **102**

Dynamical entropy and fractal dimension of laser-driven Brownian motion in strongly-coupled dust Coulomb structures

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The most interesting and practically significant open systems consist of natural and artificial active Brownian agents, i.e. particles that are able to transform an external energy into the kinetic energy of their motion. The feature of all kinds of active matter is its dynamics that differs from the behavior of passive, "classical" Brownian particles.
In present work, we have studied the dynamics of structures consisting of metal-coated dusty particles, levitating in rf-discharge plasma. The external laser radiation, acting on the metal surface, induces the

radiometric force [1]; driven by it, the metal-coated plastic particles in gas-discharge plasma should act like active Brownian agents.
To estimate the phase state of experimentally created systems, we have studied various structural and dynamical characteristics, including the dependencies of mean-squared displacement of dust grains on time on various time scales, the curves of dynamic entropy [2] and the fractal dimension of Brownian motion of structures with various values of the external laser power.

[1] Jovanovic O 2009 *J. Quant. Spectrosc. Radiat. Transfer* **110** 889–901
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The entropy and dust particle trajectory divergence in dusty plasma model

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The statistical physics, thermodynamics (entropy and thermostat model), concepts of equilibrium and partial equilibrium are crucial for dusty plasma description. The problem of estimation of dusty plasma entropy is under consideration. All approaches of this research are based on analytical and theoretical approach, and also on molecular dynamics simulation of dusty plasma system.
In the model of dusty plasmas the divergence of trajectories allows to calculate K-entropy (Krylov–Kolmogorov–Sinai entropy). The value of K is also equal to averaged maximum Lyapunov exponent and entropy growth rate since reciprocal is an important relaxation time. Furthermore, predictability time is studied. This time characterizes the time interval, during this interval future behavior of a dynamic system based on the initial conditions and deterministic dynamical equations can be predicted.

The molecular dynamics simulation shows that the time of trajectories divergence might be different in different directions, so the partial equilibrium subsystem can be observed in the system. Estimations for the characteristic time of divergence in different directions of dust particles motion are obtained. The method for entropy is estimated for conditions of standard laboratory experiment on dusty plasma. The applicability of the thermodynamic functions for the description of plasma-dust system is discussed.

Resonant energy transfer in dusty plasma

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Energy transfer between degrees of freedom of a dusty plasma system is of great interest. One of mechanisms of such energy transfer is based on parametric resonance. Its initial stages can be described by extended Mathieu equation. Molecular dynamic (MD) modeling is used to describe later stages. Model of dusty plasma system including fluctuations of dust particles charge and features of near-electrode layer is used. Using numerical approach conditions of energy transfer beginning are obtaind. Growth rates of energy and saturation energy are derived for a wide range of parameters. Obtained results are compared with results of extended Mathieu research and allow to describe energy transfer in dusty plasma more accurate.

Structures in dusty plasma in the range of temperatures 9–295 K

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This work is devoted to the study of properties of dusty plasma structures [1]. It relies on two sets of experimental data: the first one published in [2] and the second one obtained in the experiment conducted by R Kh Amirov's group in JIHT RAS in 2010–2012. In most works it is considered that interparticle distance depends on temperature like the Debye length in plasma ($\propto T^{1/2}$), in these experiments it is found that it falls faster than the square root at high temperatures and increases at cryogenic temperatures. To build a theoretical model explaining this phenomenon it is assumed that particle interaction is Yukawa-like and particles are confined in an electrostatic trap caused by ambipolar diffusion, thermophoresis, ion drag force and electric field gradient in the vertical direction. Method of molecular dynamics is used to obtain structural properties for this model. Interparticle distance dependences on the number of particles in the structure, on the particle's charge, on the trap parameter and the screening length are obtained. The influence of each force on the interparticle distance is estimated.

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[2] Polyakov D N, Vasilyak L M and Shumova V V 2015 *Surf. Eng. Appl. Electrochem.* **51** 143–51

Macroions non-linear screening in complex plasma

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The base for consideration is the well-known phase diagram of dusty plasma [1] for an equilibrium charged system with the Yukawa potential in Γ–κ plane (Γ is a Coulomb non-ideality parameter, κ is a screening parameter). There are huge negative total pressure and total compressibility areas in the initial phase diagram [1] as one uses equations of state [1] and [2] (see [3] for more details). Questions of thermodynamic stability and an existence of an additional phase transition of gas–liquid and/or gas–crystal type in two-component systems $(+Z, -1)$ and $(-Z, +1)$ are discussed. Two-component highly asymmetric electroneutral systems of classical macroions with the charge Z and point-like opposite charged microions are considered in the case of big inhomogeneity around macroions. Linear screening approximation is not valid for a considerable part of characteristic parameters of substantial dusty plasma. Poisson–Boltzmann equation is solved numerically in electroneutral Wigner–Seitz cell for two-component systems to consider non-linear screening of macroions by microions. Lateral views of microions and non-linear potentials are calculated. This allows to make charge renormalization and to consider not a real charge Z but an effective one Z^*. The work is supported by the Russian Science Foundation (grant No. 14-50-00124).

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[2] Khrapak S A, Khrapak A G, Ivlev A V and Morfill G E 2014 *Phys. Rev.* E **89** 023102
[3] Martynova I A and Iosilevskiy I L 2016 *Contrib. Plasma Phys.* **56** 432–41

Diagnostics of low temperature helium plasma of dielectric barrier discharge for medical applications

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Until recently, plasma was used only due to thermal effect. Considering of new object, called low-temperature plasma gave a lot of interesting. Electromagnetic component, chemical reactions, uv radiation and thermal effect give a synergic effect. These properties allow applying low-temperature plasma in various technical fields: medicine, dentistry, ophthalmology, food processing, biotechnology, agro-technology and manufacturing industry. It caused such high interest to this object. Diagnostics of low temperature plasma, generated by a dielectric barrier discharge were carried out in this work. Plasma generation modes depending on the various governing parameters were investigated. Generation mode has been chosen suitable for the surface treatment of living organisms in this study. Installation modes in which plasma generation was implemented were studied. There have been studies of ultraviolet radiation arising during plasma generation, it was established the safety for people. Also temperature distribution profile was measured, due to these measurements safety of the torch impact on living organisms was shown. Spectroscopic studies have shown the presence of active components contained in the plasma, such as H_2O_2, NO, NO_2, and their distribution along the torch. As well as were measured concentrations of some of these components (NO, NO_2). These studies are of particular interest, because they provide new information in this area. The received results allow optimizing various parameters of physical plasma for applying in various biological fields.

Correlational approach to study interactions in complex plasmas

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One of the important experimentally unsolved problems in complex plasmas is a spatial structure of the wakefield (a result of interaction of microparticles with a plasma flow). Since the wake is formed behind the particle downstream the ion flow, a flow-aligned particle chain in a plasma-sheath is a convenient structure for studying the wake-mediated interaction between particles. In this work, we present a new contactless technique for studying pair interactions in complex plasmas based on measuring the time-averaged correlations of particles displacements and velocities. We derive simple analytic equations, which allow one to calculate the gradients of forces acting on the particle due to each of the other particles as well as the gradients of external field, knowing only the values of the above correlators. In the examples of numerical simulations, we show that the proposed approach could be an effective instrument in exploring the wake of a dust particle. Unlike the previous attempts to study the wake-mediated interactions in complex plasmas, our method does not require a special design of the experimental setup, does not need the help of gravity and special laser manipulations, and therefore can be applied in microgravity experiments (e.g. in the PK-4 facility, recently delivered to the ISS).

Energy exchange in the systems with non-uniform thermal sources

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Processes of an energy exchange in the systems of interacting grains with non-uniform spatial distribution of thermal sources and (or) any other sources of stochastic kinetic energy are considered. For the first time the theoretical model for the analysis of energy balance in dissipative systems is proposed. On the basis of this model the analytical relations for the redistribution of "kinetic temperature" between the charged grains are found. The obtained relations were tested by numerical simulations of the problem for Yukawa systems. The results of presented study can be useful for analyzing the energy exchange in inhomogeneous systems with any types of reciprocal interactions, which are of interest in plasma physics, medicine, biology, and the physics of polymers and colloidal systems.

Self-assembly of particle pairs in complex plasmas

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For particle coupling (at condensation and self-assembly of so-called dust molecules) to occur in the dust subsystem, there must be attractive forces between dust particles. The question of attraction between two like-charged (dust) particles in plasma medium has been a hot topic for the past 20 years. The Boltzmann–Poisson model framework does not allow for two particulates with the same charges immersed in plasma to attract each other. Nevertheless, there are

many mechanisms which can lead to an effective attraction for two like-charged particles in plasma. For example, shadowing forces in isotropic homogeneous plasma or effects of ion focusing in a flowing plasma. Thus far, there is no experimental observation of dust grain pairs, which are self-confined by wake-mediated attraction.
In this work, we present the results of analytical and numerical study of the existence of self-confined particle pairs in complex plasmas. We call a system self-confined when the stability of its bound state is not provided by external fields, but is provided by attraction between particles. We obtained the stability conditions of the pair (bound) state depending on the interaction parameters and particle kinetic energy. To illustrate the results we used a modification of the point-wake model of interparticle interactions in an anisotropic plasma. It was shown that the breakup of the particle pair is very sensitive to the ratio of particle charges, which can be different from the unit, for example, due to decharging of the lower particle caused by the influence of the upper particle on the ion flow. We also showed that a self-confined pair of particles exists even if their total kinetic energy is much greater than the potential well depth for the pair state. This occurs due to velocity correlation of particles, which arises with the non-reciprocity of interparticle interaction.

Numerical simulation of dust particle in weakly ionized plasma in collisional regime with the finite difference lattice Boltzmann method

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The problem of dust particle charging in collisional regime is of interest for complex plasma study [1]. In this work we present a numerical method for simulation of plasma around dust particle in collisional regime. This method is based on FD-LBM (finite

difference lattice Boltzmann method) scheme which replaces Euler–Poisson equations for weakly ionized gas. This method allows refining results obtained by means of drift-diffusion approximation, because the incorporation of convective term (as opposed to the drift-diffusion approximation) could significantly change the current through particle surface and, therefore, change particle charge too. The use of straightforward kinetic boundary conditions for perfect absorption allows us to calculate the non-zero concentration near the probe surface without any additional assumptions about flow structure, unlike other commonly used boundary conditions for full absorption. In this article, we demonstrate the results of our simulation (spatial and temporal distribution of plasma density and flow, charging process) in a wide range of plasma parameters (collisional regime) and compare them with existing results of the numerical and analytic models of other authors.

[1] Fortov V F and Morfill G E 2010 *Complex and Dusty Plasmas: From Laboratory to Space* Series in Plasma Physics (Boca Raton, FL: CRC Press)

Screening dust particle charge in an *e*-beam created humid air plasma

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A kinetic model has been developed for charged particle reactions in humid air plasma produced by fast electron beam. The model includes over 550 reactions with electrons, 33 positive ion species and 14 negative ion species. The model has been tested by solving 48 non-steady state equations for number densities of charged particles in the humid air *e*-beam plasma, and comparing with the available experimental data.

The system of 48 steady state equations has been solved by iterative method in order to define the main ion species of the humid air plasma. A reduced kinetic model has been developed to describe the processes with the main ions and electrons. The screening constants have been calculated on the basis of the reduced system by means of Leverrier–Faddeev method. The dependencies of the screening constants on gas ionization rates have been found for the rates from 10 to 10^{18} $cm^{-3}s^{-1}$ and the fraction of water molecules from 10^{-6} to 2%. The analysis of the constants has revealed that one of them is close to the inverse Debye length, and the other constants are defined by the inverse diffusion lengths passed by ions in the characteristic times of the attachment, recombination, and ion conversion. Pure image screening constants appear at low rates of gas ionization.
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Dusty waves and vortices in rf magnetron discharge plasma

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The appearance and subsequent growth of particles in rf magnetron plasma over the flat sputtered electrode were observed. In some regions the particles were involved in the horizontal or vertical vortex movement. The horizontal rotation along the sputtered track in the cyclotron drift direction was observed close to the main magnetron plasma. Another vortex ring of submicron particles engirdled the secondary plasma of the discharge at height of a few centimeters over the electrode. Close to this region particle density waves propagated through the cloud. The possible role of discharge

plasma azimuthal inhomogeneity and gas dynamics effects in the forming the observed structures was considered.
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Effect of interelectrode distance on dc magnetron discharge characteristics

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We investigated planar direct-current magnetron discharge in the sputtering system equipped with movable anode. Current–voltage and current–pressure discharge characteristics were obtained varying the anode-cathode distance in the range of 10–150 mm. The corresponding changes of ion spatial distributions were studied using optical emission spectroscopy. It is found that decreasing the distance from 80 to 10 mm results in decrease of dc magnetron discharge current. The current–pressure characteristics have a local maximum that become less pronounced and shifts toward the higher pressure as the distance decrease. The explanation of the obtained results is given.
The work was supported by the Russian Science Foundation (project No. 16-12-10511).

Pre-breakdown characteristics of weakly ionized liquid and gaseous media in the electric field of the high-voltage edge

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By solving the system of equations [1] of the pre-breakdown charge formation in quasi-neutral media such as transformer oil, derived earlier by the first author of this work, quasi-exponential formula of the current-voltage characteristics of low conductive dielectric fluids in the high-voltage electric fields of a spherical capacitor and a needle electrode was analytically obtained. Also from this system of equations a linear dependence of the radius of the microbreakdown zone in the vicinity of the edge of the needle electrode on the applied dc voltage was obtained. For the analysis of the pre-breakdown characteristics of weakly ionized gaseous media such as air in discharges in the vicinity of the high-voltage edges it is inappropriate to use the aforementioned system of equations. Therefore, for such conditions an experimental study was carried out. Empirical current-voltage characteristics similar to the quasi exponential were obtained. The dependence of the size of the microbreakdown zone on the applied voltage was close to linear. The analysis of the obtained results was carried out. The scheme of the experiments is presented.

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Forced oscillations of the Coulomb structure in the linear electrodynamic trap

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Electrodynamic traps are convenient tools for studying the properties of individual charged particles as well as Colulomb strutures formed by hundreds and thousands of these particles. The excitation of oscillations of charged particles confined in the linear electrodynamic trap is presented. The trap consisted of four cylindrical horizontally oriented electrodes. The oscillations were excited by rectangular electric pulses applied to the additional electrodes, which were located at the ends of the trap. The pulses amplitude was varied from 10 to 320 V. The pulses frequency was varied from 0.1 to 100 Hz.

We used a polydisperse Al_2O_3 powder. The particles charging was carried by the induction method. The particles were placed on a metal electrode. The electrode was moved to the trap and the particles were drawn into the interelectrode space.

By increasing the frequency of the electrical the pulses, the amplitude of the oscillations was reduced. At the frequency of 20 Hz the oscillations practically stopped. The analysis of the oscillatory motion allowed us to determine the mean particles charge.

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The ordered structures of dust particles in a dynamic linear trap with the corona discharge generated by an alternating electric field

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The aim of this work is to study the possibility of capturing and confining of particles in a linear electrodynamic trap with corona discharge generated by an alternating electric field at atmospheric pressure. The electrodynamic trap consisted of four cylindrical horizontally oriented electrodes. The electrodes length was equal to 10 mm and the electrodes diameter was equal to 300 μm. The distance between the electrodes was equal to 10 mm. Corona discharge between the electrodes ignited at a voltage of 3 kV. The ac voltage frequency was equal to 50 Hz. Trajectories of the particles were registered by CCD camera HiSpec 1. Illumination of the particles was provided by a 532 nm laser. We used a polydisperse Al_2O_3 particles with a size of 10–40. The particles were injected into the trap from the top side. The particles were charged up in an electric field of the corona discharge during downward motion and were captured by the trap, forming an ordered structure near the axis of symmetry of the trap.

The possibility of capturing and confining of the ordered Coulomb structures in the linear electrodynamic trap with the corona discharge generated by an alternating electric field at atmospheric pressure was experimentally demonstrated for the first time.

Coulomb structures in the annular electrodynamic trap

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Electrodynamic Paul traps and their modifications were used for confining of levitating charged particles. Polydisperse Al_2O_3 particles were confined in a linear quadrupole electrodynamic trap in air at the atmospheric pressure [1]. In [2] the force acting on the particle in the trap of finite length was studied. It was shown that confining potential occurs at the ends of the trap and the electric field is substantially inhomogeneous. Furthermore the field is not enough to form Coulomb structures with a large number of particles. In [3] multi-electrode traps were studied.

In this paper we used an annular electrodynamic trap to eliminate inhomogeneity of the electric field. The trap consisted of four annular electrodes with a diameter of 12 and 16 cm. The distance between the electrodes was equal to 2 cm.

The experimental results are presented. The particles were formed a toroidal structure along the axis of the trap.

This work has been supported by the Russian Science Foundation grant No. 14-50-00124.

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Photoelectric determining of the microparticles sizes in separation processes

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The paper presents the method for particle size diagnosis by analizing of the scattered laser radiation on them. The method uses the light scattering Mie theory and the approach presented in [1]. Illuminating particles with laser of known radiation density and using photocamera of known parameters (the aperture size, the dependence of the spots brightness on the image from the laser beam of known power) one can determine the diameter of the particles in the assumption spherical shape. The method was verified at 3 types of monodisperse particles of melanin formaldehyde. The obtained sizes were compared with sizes measured by the microscope. The resulting linear relationship between sizes form method and gained from microscope allowed using of this method for the diagnosis of particle sizes in the processes of particle separation. The work was done under financial support from the Russian Foundation for Basic Research (grant No. 16-32-00031).

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Formation of dust-acoustic waves in the plasma of the protons beam

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The results of the experiments performed at the electrostatic accelerator EG-2.5 of the Physical-Power Institute are presented. The experimental cell used for the experiments has been described in several works (for example, [1]). But we made some insignificant changes concerning a measurement of pressure of the plasma forming gas. The main characteristics of the gas–dust mixture are as follows: gas is He, pressure is 0.78×10^5 Pa, dust particles are CeO_2, current of protons is 1 μA, energy of protons after a flight through a foil dividing a high-vacuum target conductor and experimental cell is 1.5 MeV, voltage at the high voltage electrode is 500 V. The protons beam is a horizontal one. Firstly, the dust–gas cloud was registered with the help of a digital camera at the voltage applied to the electrode but when the proton beam was closed (by a gate in a target conductor). In this case the non-disturbed motion of dust particles in the cloud was observed. Then, when the gate was opened, in the vicinity of the high-voltage electrode the dust acoustic waves were excited. The exited waves were propagating under an angle to the parallel beam of protons. The following parameters were measured: wavelength $\lambda = 0.6$–0.8 mm, velocity of the wave propagation is $v = 12$–19 mm/s. These parameters correspond to the dust-acoustic waves.

Changes in the surface structure of melamine-formaldehyde particles in complex plasma

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A glow discharge plasma of inert and molecular gases is widely used for surface modifications of polymer materials. Films, fibers or microparticles placed in the plasma acquire new physical and chemical properties, and their sizes often change.
The use of complex (dusty) plasma in this context has hardly been studied [1, 2]. Microparticles placed in discharge become a part of a stable plasma–dust structure. The effects of plasma fluxes on the surface cannot be assessed by means of optical methods while particles are in the discharge, nor after collection of modified particles from the discharge chamber. Scanning electron microscopy gives information about changes in the sizes and surface topography of microparticles exposed to the complex plasma for a certain time. This paper presents the results of a study of the surface modification of calibrated spherical particles of melamine-formaldehyde, occurring in ordered dust structures in the plasma of a neon glow discharge. We describe the technology for generating complex plasma, the method for collecting particles from it, the procedure for studying the changes in the surface of particles using electron microscopy, and the analysis of data.

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Potential distribution around charged particle in a collisional weakly ionized plasma in an external electric field

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A pointlike absorbing charged particle in uniform anisotropic plasma with an external field $\mathbf{E}_0$ is under consideration. The ion and electron motion is described in drift-diffusion approach with variable mobillity. Small perturbations for plasma parameters are considered. For the important case of $T_\mathrm{e} \gg T_\mathrm{i}$ (T_e and T_i are temperatures of electrons and ions) the Fourier transformed additional potential is

$$\varphi(\mathbf{k}) = \frac{Q\left(\mathbf{k}^2 + i(\mathbf{k}\mathbf{k}_\mathrm{E})\right) + Q_\infty k_\mathrm{D}^2}{(2\pi)^{3/2}\epsilon_0\left(\mathbf{k}^4 + i(\mathbf{k}\mathbf{k}_\mathrm{E})\mathbf{k}^2 + k_\mathrm{D}^2\left(\mathbf{k}^2 - \eta(\mathbf{k}\mathbf{k}_\mathrm{E})^2/\mathbf{k}_\mathrm{E}^2\right)\right)}, \quad (1)$$

where Q is the charge of the particle,$Q_\infty = -J_\mathrm{d}\epsilon_0/(\mu_\mathrm{i} n_\mathrm{i})$, where J_d is a plasna flux on the particle, μ_i and n_i are mobillity and ion number density, k_D is inversed Debye radius, $\mathbf{k}_\mathrm{E} = e\mathbf{E}_0/(k_\mathrm{B}T_\mathrm{i})$, and $\eta = |\mathbf{E}_0|/\mu_\mathrm{i}\partial\mu_\mathrm{i}/\partial|\mathbf{E}|$. For the large distances (small k) the asymptotic expression is valid:

$$\varphi(\mathbf{r}) \approx \frac{Q_\infty}{4\pi\epsilon_0 r'} - \frac{(Q - Q_\infty)(\mathbf{r}\mathbf{k}_\mathrm{E})}{4\pi\epsilon_0 k_\mathrm{D}^2 r'^3} + \frac{3\eta Q_\infty(\mathbf{r}\mathbf{k}_\mathrm{E})\left(\mathbf{r}^2 - (\mathbf{r}\mathbf{k}_\mathrm{E})^2/\mathbf{k}_\mathrm{E}^2\right)}{8\pi\epsilon_0 k_\mathrm{D}^2 r'^5}, \quad (2)$$

where $r' = \left(\mathbf{r}^2(1-\eta) + \eta\frac{(\mathbf{r}\mathbf{k}_\mathrm{E})^2}{\mathbf{k}_\mathrm{E}^2}\right)^{1/2}$. The first term corresponds to Coulomb–like potential in isotropic plasma [1]. The second term describes polarization of the ion cloud. In the weakly collisional conditions Q_∞ comes to zero, η is 0.5 and second term consists with the result of the kinetic approach [2].

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Numerical study of the parameters of low-pressure glow discharge in argon at the organization of acoustic streaming

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Low-temperature plasma has been widely used in various fields of modern science and technology: modification of the surface of materials, plasma spray coating process, powerful light sources, the semiconductor industry (production of microchips), space electric rocket engines. The ability to control the discharge structure, as well as flow and concentration of charged and excited particles [1] is of special interest. In this study, within hybrid model of the discharge [2] in argon at low pressures, demonstrated the possibility of controlling the parameters and structure of a glow discharge through the organization of acoustic streaming in the discharge tube when excited in her a standing acoustic wave. It is shown that the acoustic flow may be the main reason for the discharge reduction in a standing sound wave field. At the same time achieving the necessary sound pressure values at which the speed of acoustic streaming is comparable to or greater than the flow of ions caused by drift in an electric field and diffusion they can be increased concentrations of charged and excited particles in the axial region of the discharge. However, he remains stable, as evidenced by the growing nature of the current-voltage characteristics.

This work was supported by the President of the Russian Federation (grant No. MK-539.2017.1) and the Russian Foundation for Basic Research (project No. 16-38-60187).

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Displacement of the border of transition to normal glow discharge in neon at cryogenic cooling

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The studies of electrical characteristics of gas-discharge plasma cooled to cryogenic temperatures are necessary for the study of processes in dusty plasmas and are motivated by the ability to create a new class of cryogenic plasma chemical technologies [1, 2]. We investigated the electrical characteristics of the dc discharge in neon at the border of transition to the normal glow discharge at cryogenic (77 K) and room (295 K) temperatures of the gas at a pressure from 18 to 187 Pa. The gas pressure in the discharge was maintained constant when the temperature changed. In the process of cooling the dependence of the electric field strength on the temperature was determined by the magnitude of the discharge current. Upon cooling of discharge with a discharge current corresponding to the normal regime at a given pressure, the electric field always increased with decreasing temperature. With a discharge current corresponding to the subnormal regime, the electric field in a certain temperature range decreased and there was a change in a regime of the discharge with decreasing temperature. It has been found that At cooling, the boundary of transition to the normal regime shifted to lower currents. Despite the fact that at cooling the electric field at the boundary of the transition to normal discharge increased, the value of the reduced electric field decreases in the entire range of current and discharge pressure. This work was supported by the Russian Foundation for Basic Research grant No. 16-02-00991.

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Transformations of dusty structure in cryogenic dc discharge in neon

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Effect of discharge current on a shape of the dusty structures in a dc discharge in neon at cryogenics (77 K) temperature and for pressure of 0.14 up to 1.4 Torr is experimentally investigated. At temperature 77 K, the increase of the discharge current leaded to the reduction of the longitudinal and increase of the radial dimension of the dust structure as it was previously observed at room temperature [1]. The decrease in gas pressure resulted in a decrease in the density of the dust structures and initiation of oscillations and vortex motion of dust particles at the periphery of the dust cloud. In the normal glow discharge, the decrease of the current at low pressure resulted in increased deviations of the dust particles from the equilibrium position. Under the transition into the subnormal mode, the increasing of a longitudinal electric field leaded to the formation of the ordered dust structures and to the formation of the complex clusters [2]. For spherical dust structures was revealed a value of the minimum of function for dependence of wattage per unit length of discharge from a pressure. The growth of this function at increasing pressure is mainly determined by the losses on the dust structure associated with increasing of size and the dust particle density [3]. The decrease of this function at low pressure is determined by the size of the dust structure associated with the motion of dust particles. This work was supported by the Russian Foundation for Basic Research grant No. 16-02-00991.

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Model for grounding electrode characterics

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Experimental investigations of nonlinear processes of spreading of the pulse current in soil in the laboratory and on the high voltage testing area for a single electrodes in the form of a sphere, rod, disk. The process of the pulsed current spreading at current densities greater than the critical value leads to a sharp non-linear decrease in pulse resistance as a result of ionization and sparking in the soil near the electrode. I–V characteristics and dynamic resistance of ground electrodes of large dimensions with various geometric shape and the same surface area were obtained on the high-voltage testing area. It is shown that the geometric dimensions of the earthings have a great influence on the value of they dynamic resistance. At equal surface area and equal of the voltage pulse amplitude earthing rod with a length of 4.8 m has the smallest dynamic resistance, and the highest–hemisphere with a diameter of 34 cm, which is due to increased inhomogeneity of the electric field at the electrode surface. On the basis of the obtained experimental data, a dynamic equivalent circuit of the earthings and proposed a model of grounding electrode taking into account spatial sparking in the soil, differs from previously proposed models that in addition account for the symmetric and uniformly distributed zones sparking taken into account non-uniform distribution of the sparking zone with the accounting for the formation of localized extended plasma channels, leading to an increase in the effective length of earthing. The results of the calculation by this model shows good correlation with the experimental data.

Excitation of magnetic dipoles in dielectric ring by plane transverse electromagnetic wave

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Our experimental investigations of resonant phenomena in the electromagnetic fields generated by displacement current in the near zone of dielectric ring in the rf range radiation were carried out. The experiments were carried out at the excitation of lower resonant frequencies in the dielectric rings irradiated by the linearly polarized microwaves. Agilent E5071C ENA Network Analyzer was used for the generation and registration of emission spectra of GHz-range. Dielectric ring with square cross-section used in these experiments is characterized by the dielectric permeability value of 200. It's external radius is 1.9 cm, thickness is 0.5 cm. Two different arrangements of the ring with respect to the vector of electric field and magnetic field components of the incident wave were examined. The measurements of electric field, generated by the displacement current in the ring, were performed for two cases. Case 1-polarization structure of incident wave; plane of the ring is perpendicular to the wave vector Observation of scattering on this ring had revealed the lowest resonant frequency near 15 GHz. Case 2-plane of the ring is perpendicular to the magnetic component of the incident wave. The spectral measurements had revealed the novel the lowest resonance at the frequency value of 1.36 GHz. Experimental value of resonant frequency is in good agreement with the theoretical value found by us. Herein the half bandwidth of this resonance 20 MHz indicates the low losses in the dielectric ring, ensuring the possibility to use this effect in creation of new single-negative metamaterials with negative magnetic permeability. The results of our research give the opportunity to create new metamaterials with low loss of energy based on high-frequency ceramics.

Microbubbles influence on the discharge development in conductive liquid

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An influence of air microbubbles regularly distributed in conductive water on the discharge parameters, such as breakdown voltage and timelag has been studied experimentally in relatively short gaps at strongly non-uniform electric field. The experiment parameters were as follows: applied voltage, kV: 3–4; voltage pulse risetime, μs: 1; pulse duration (FWHM), ms: 5; gap distance, mm: 1; electrodes geometry: pin-to-plate (anode–conic shape, 1.7 mm height, 1.6 mm diameter, 100 μm tip diameter; cathode–1.6 diameter plate with rounded fillet); water conductivity, μS/cm: 300; volumetric gas content range, %: 0.1–3; microbubbles Sauter mean diameter, μm: 59. Degassing of preliminary pressurized water through cylindrical output nozzle was used in order to obtain liquid with regularly distributed microbubbles. Microbubbles size distribution was controlled by means of shadow images statistics. Volumetric gas content ϕ was calculated with the assumption of isotropic spatial bubbles distribution basing on the 2D images. In order to obtain gas volumetric content evolution in time the sets of 10 images (10 sets of 10 images) were processed separately giving us the dependence ϕ(t). The experiments were conducted for the four different values of volumetric gas content (in %): 0, 3.0, 1.5, 0.2. Captured waveforms and shadow images revealed neither breakdown voltage nor the timelag to breakdown to depend on ϕ in conditions of strongly non-uniform electric field and short gaps. At such applied voltage the discharge initiation follows the thermal mechanism. The presence of microbubbles on the electrodes surface and in a bulk liquid doesn't affect the mechanism of discharge development.

The spatial structure of the barrier discharge in air

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An investigation of the spatial structure of the barrier discharge, using high-speed video camera with the image intensifier and the microscope allows obtaining high spatial resolution. The voltage of barrier discharge was 7 kV. Spatial analysis was based on images averaging during the same phase of the discharge, for streamer phase of the discharge it is first quarter of the period. Obtained that the highest brightness of the radiation occurs in the narrow, not more than 100 μm, near-electrode layer. The maximum energy in the discharge gap is embedded in a region at distances of 50–250 μm from the high voltage electrode. The most effective generation of the active particles takes place in a wider region of the discharge at a distance of 100–600 μm from the high voltage electrode. Preliminary studies of the effect of germicidal uv radiation were carried on bacteria Staphylococcus aureus, which were in a drop of physiological solution on the surface of the polyvinyl chloride plate. The results of the evaluation of the disinfection of surfaces germicidal uv-radiation showed that, at the dose of 1.2 J per square meter the efficiency of disinfection amounted to 99.99%. Based on the results obtained, as well as, evaluation of electric power in the electrode gap of the barrier discharge one can assume comparable results of disinfection can be obtained in a comparable or less treatment time of test using barrier discharge with an equivalent electric power.

Mathematical modelling of radio frequency plasma flow with metastable atoms at low pressure

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Radio frequency (rf) plasma at low pressure ($p = 5 - 150$ Pa) with gas blowing is effectively used to modify the surfaces of materials of inorganic and organic nature [1]. Plasma of this type has the following properties: electron concentration 10^{15}–10^{19} m^{-3}, degree of ionization is 10^{-4}–10^{-7}, 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 rf plasma neutral component stream is in a transitional mode between the continuum mode and free-molecule flow, the electron component can be approximated of continuous medium [2]. Mathematical model of rf plasma flow at low pressures with influence of metastable atoms is constructed. Calculations of rf plasma flow at low pressure are completed. The distributions of the velocity modulus, pressure and temperature of the carrier gas and the electron concentration, electron temperature, metastable concentration are obtained. The reported study was funded by Russian Foundation of Basic Research, according to the research project No. 16-31-60081.

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Influence of the length of the actuator on the parameters of dielectric barrier discharge and thrust of the synthetic jet

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To control the low-speed high-altitude unmanned aerial vehicles (UAV), which do not require high maneuverability, actuators based on dielectric barrier discharge (DBD) can be used as a single flight controls. Works devoted to dielectric barrier discharge had the size of DBR actuator do not exceeded 100 mm [1-3]. The real high-altitude UAVs have a wingspan of about several meters. It raises the problem of scaling of laboratory results to designed vehicles.

Investigation of the excited state population density of electric propulsion thruster plasma in 3D by laser induced fluorescence

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At preset paper the excited state concentrations distribution of a thruster with closed electron drift at 300 W operating conditions low-temperature xenon plasma was investigated by laser induced

fluorescence (LIF) in the 350–1100 nm range. More than 15 xenon ions (Xe II) transitions were analyzed, while for neutral atoms (Xe I) just few transitions were explored. The reason is that the majority of Xe I emission occurred in the ultraviolet or infrared part of the spectrum which is difficult to measure. The necessary spontaneous emission probabilities (Einstein coefficients) for xenon atom were calculated at the Coulomb approximation (800 transitions). Measurements of the excited state distribution were made for points (volume of about 8 mm^3) all over the plane perpendicular to thruster axis in five positions on this axis (5, 10, 50, 100, 200 mm). Measured LIF signal intensity have differences for each location of researched point (due to anisotropy of thruster plume), however the structure of state concentrations distribution persisted. Measured distribution show that plasma of thruster with closed electron drift can not be described on the assumption of local thermodynamic equilibrium or Coronal model. Collisional-radiative model applicability varies for different measurement positions (in 3D) and selected transitions.

On the calculation of dynamic and heat loads on a 3D body in a hypersonic flow

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We are considering a 3D body in a hypersonic flow with zero angle of attack. The aim of the paper is the estimation of heat and aerodynamic loads on specific body elements. We are considering a previously developed code to solve coupled heat- and mass-transfer problem. The change of the surface shape is taken into account

by formation of the iterative process for the wall material ablation. The solution is conducted on the multi-GPU cluster. Five Mach number points are considered, namely for M = 15–19. For each point we estimate body shape after surface ablation, heat loads on the surface and aerodynamic loads on the whole body and its elements. The latter is done using Gauss-type integration on the surface of the body. The comparison of the results for different Mach numbers is performed. We also estimate the efficiency of the Navier–Stokes code on multi-GPU architecture for the coupled heat and mass transfer problem.

Supersonic plasma jet in the experiments on radiophysical testing flow bodies

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To date, the plasma jet obtained by magneto-plasma compressor (MPC) and a pulsed discharge in capillary with ablating wall actively studied in various experiments. Earlier, we noted that these relatively simple sources can be effectively used in applications of magnetoplasma aerodynamics. The speed range of such plasma jets is 0.5–10 km/s, and the duration of the working cycle can vary from 50 μs to a few tens of ms in the range of static pressures of the air 10–500 Torr. So the plasma flow processes of the different models was started, including the study of the influence of the direction and magnitude of the magnetic field on the characteristics of the flow inhibition zone. Were also conducted the first experiments for the study of radiophysical properties of such jets. It was found that the location on the body surface of the magnetic field source of a specific orientation leads to an increase in the departure of the shock wave

and the weakening of the intense luminescence zones of the ionized gas in this region. It is confirmed that the strong attenuation of the mm-cm-microwave radiation (2 dB), observed in the inhibition zone at zero magnetic field, is significantly reduced when a magnetic field of specific value and orientation is applied.

Propagation of microwave radiation through an inhomogeneous plasma layer in a magnetic field

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The 1-D model is proposed, which allows to consider the propagation of electromagnetic waves through nonuniform magnetized plasma layer. The results of calculations of the transmission and scattering coefficients of EM waves in the centimeter range at various values of the magnetic field where presented. It is shown that the amplitude of the reflected signal increases weakly with increasing magnetic field. The transmission coefficient reaches maximum levels at values of the magnetic field exceeds 0.7 T. The results of experiments in which the microwave radiation passes through the plasma layer of microwave or pulsed high-voltage discharges will also present.

Investigation of poor propane–air mixture ignition by microwave discharge

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In numerous experiments it demonstrated the possibility organization of working process using the microwave plasma generators to initiate the surface and volume plasma discharges in areas of flow before the tear zone and therein to stabilize the flow in the model channel tested in free flow, and under the attached air duct. The use of microwave generators to initiate plasma discharge caused by a number of advantages. Almost all other types of electrical discharges in gases have low efficiency power supplies energy investments in the discharge. High energy efficiency of microwave discharge is a major advantage in creating such ignition systems in the combustion chambers and jet flight control systems. Using the microwave plasma formations for heating the working gas at relatively low pressures may be preferable because thus realized tied deeply subcritical streamer discharge and the area of impact on the gas mixture is wider than the spark. This is especially important in the case of the organization of the combustion of lean mixtures in composition close to the limits of ignition and combustion. The use of microwave energy increases the range of possible application of an external energy supply in order to organize the working process in industrial power plants and propulsion systems of aircraft. The aim of the test was to measure the gas-dynamic flow parameters and initiation of ignition of flammable poor mixtures by a microwave discharge. The object of the test is selected cylindrical flow working part installed on a test bench MRTI RAS, with installed linear cylindrical vibrator.

Distributed plasma system for ignition and flameholding in supersonic flow

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The plasma systems for ignition and flameholding are studied sufficiently well in laboratory conditions. At the present time stable operation over a wide range of gas temperatures and Mach numbers are shown [1]. The main disadvantage of this method at present is a high power consumption, which limits the use of plasma generators in real apparatuses. This devoted to experimental study of ignition and flameholding in supersonic flow by means of distributed plasma system, which allows extending the life of the electrode system, and reducing the total energy consumption due to the flexible circuits and, in the long term, the use of feedback. Two rows of electrodes were flush mounted to the ceramic wall downstream of the injectors for gas fuel (ethylene). Both electrode systems were powered independently via two fast high voltage switches. Following series of experiments were provided with ignition and flameholding at varying of fuel flow rate and electrical power of discharge: 1) the use of only first electrode system 2) the use of only second electrode system 3) use of both systems, but first one was used only short time for ignition 4) use of both systems, but second row of electrodes was used only short time for ignition. These experiments are currently ongoing. The preliminary results let us suggest that the case (3) seems to be the most effective. This work is supported by Russian President Grant for young scientists MK-1734.2017.8.

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Radiation transport in the channel of the quasi-steady plasma accelerator

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The study of the axisymmetric ionizing gas flows in a channel of the quasi-steady plasma accelerator is presented. Model is based on the magnetohydrodynamic (MHD) and radiation transport equations. The modified MHD model for a three-component medium consisting of atoms, ions and electrons takes into account the basic mechanisms of the electrical conductivity and heat transport. The model of the radiation transport includes the basic mechanisms of emission and absorption for the different parts of the spectrum. Results of the numerical studies of ionization process and radiation transport are obtained in the approximation of the local thermodynamic equilibrium. This research was supported by the Russian Science Foundation (grant No. 16-11-10278).

Application field and ways to control ac plasma torch with rail electrode

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Recently there has been arouse interest in the creation of environmentally sound waste treatment technologies on the basis of plasma torches. At high temperatures in furnaces and especially in plasma-chemical reactors, chemical processes flows at very high rates and do not limit the speed of the summary process [1]. The principle

of electrodynamic arcs movement in their own current field (railgun effect) is the basis of operation of plasma torches with rail-type electrodes [2,3]. Fast movement the arc attachment point along the electrode under the influence of electro-gas-dynamic forces distributes the heat load along the length of the electrode. One of the main advantages of the plasma torches is sufficiently low voltage level on the main electrodes. Supply: voltage—380–480 V, frequency—50–60 Hz. A part of the plasma generator includes a single-phase high-voltage plasma torch as an injector of charge carriers. Its power is 5–10 kW, the plasma working gas flow rate is 2–5 g/s. Efficiency depends on operating conditions and can reach 0.85. These plasma torches can operate with a wide range of gases. The task of managing the movement parameters of the main arc by changing the parameters of the injector plasma jet has been solved (filling of the chamber).

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Plasma injector for a three-phase plasma torch with rail electrodes

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The main technical feature of this type of plasma torches is rod electrodes [1] located in cylindrical channels. The electrode consists of two elements: insulator and tip. The main feature of the tip is assurance of the stable operation of the plasma torch with a long lifetime. The gap between the wall of the cylindrical channel and

the tip region is selected based on the condition of self-breakdown. The electrode is designed so that between the sealing bushing and the region of maximum diameter of the tip there is a space with a smaller diameter. This cavity acts as a vortex chamber into which the working gas is fed from the tangentially drilled hole in the wall. Operation of the ac plasma torch [2, 3]: high ac voltage is applied between the channel wall and the electrode tip. In the area of the minimum distance between them there is the electrical breakdown. The initiated arc under the influence of gas-dynamic and electrodynamic forces moves toward the nozzle. The arc is elongated in the radial direction, then when one of its attachments reaches the electrode end, another moves along the channel wall and is further at its outer end edge, where it is closed in the air with the arc of another channel. Technical parameters: supply voltage 6–1 kV; arc voltage drop 1100–1300 V; arc current up to 10 A; plasma forming gases—air, argon, CO_2; gas flow rate from 1 to 6 g/s.

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The reaction of chlorobenzene with plasma of H_2O, CO_2, CH_4 obtained by an ac plasma torch with a vortex stabilization

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Chlorinated waste is a major environmental problem, because their thermal treatment leads to the formation of dioxins. The main

possible methods of processing are direct combustion, catalytic reduction, plasma methods. Heat provided by the electric arc and water vapor may increase conversion chlorine compounds and reduce the emissions of dioxins. In this paper we consider a three-phase ac plasma torch with a vortex stabilization of the arc. The plasma torch has two input zones plasma-forming environments: near the electrodes and the arc zone. In the electrode zone is supplied shielding gas and the arc zone is fed steam, methane and chlorobenzene vapor. Chlorobenzene is selected as the most simple chlorine-containing aromatic compound having a boiling point of 131C. The resulting products were analyzed by mass spectrometry, XRD, scanning electron microscopy, differential thermal analysis, IR spectroscopy. The gaseous and liquid fractions was able to detect only one chlorine-containing compound (HCl). However, soot yield was 1.31 by weight of the raw materials, and the chlorine content in the soot—1.61. The IR spectra confirmed the linkage Cl-O and Cl-C. On the tips of the electrodes are protected with carbon dioxide, chlorine-containing compounds were observed.

Effect of electronegative additives on physical properties and chemical activity of gas discharge plasma

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Effect of electronegative additives (oxygen O_2, sulfur dioxide SO_2, carbon disulfide CS_2, and carbon tetrachloride CCl_4) on physical properties and chemical activity of plasma formed by streamer corona and by non-self-sustained discharge supported by pulsed electron beam in atmospheric pressure gas mixtures was investigated. Experiments and calculations show [1] that addition of 0.02–1.6% of SO_2 to an atmospheric pressure air leads to a decrease in amplitude of non-self-sustained discharge current supported by an electron beam of 50 μs duration by 1.5–5 times because of intense attachment of electrons to sulfur dioxide.

It was shown that with the use of streamer corona discharge of 20 ns duration an addition of 10–20% of O_2 to an atmospheric pressure nitrogen did not lead to a significant decrease in discharge current amplitude. However, an addition of 1% of CS_2 led to a decrease in the discharge current amplitude by 3 times [2]. Moreover, an addition of 1% of CCl_4 gave a decrease in the discharge current amplitude by about 10 times. The reason is the difference in rate constants of electron attachment processes for the above molecules. In experiments on volatile organic compounds (VOCs) conversion in air by streamer corona it is obtained that an addition of CCl_4 both decreases the discharge current amplitude and increases the VOCs conversion degree. The result is a significant decrease in specific energy expenditures for VOCs removal.

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Modeling barrier microdischarge at different signals of supply voltage

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In this work modeling of atmospheric pressure barrier discharge in argon for various types of voltage signals applied to the electrodes was conducted. The model included balance equations for the densities of charged (electrons, ions) and the excited particles, the electron energy density, and the Poisson equation for the electric potential. The fluxes of charged (electrons, ions) and electron energy flux were given in the drift-diffusion form. We considered two types of signals applied to the electrode with various frequency: sine wave signal and square wave signal with duty ratio variable. In the simulation result was obtained spatial-temporal distribution

pattern parameters of dielectric barrier micro-discharge at atmospheric pressure. It has been shown that there is a current pulse at half period the voltage supplied to the discharge for the conditions of the discharge and the account number of plasma chemical reactions occurring in the discharge. Graphs the distribution of the main dielectric barrier micro-discharge parameters are presented in moments of current pulses with different polarities. The described model of allows us to describe the main parameters of dielectric barrier micro-discharge plasma at atmospheric pressure and it is a useful tool in predicting their basic properties under various external conditions. This work was supported by the Russian Federation Presidential Grant (project No. MK-539.2017.1) and the Russian Foundation for Basic Research (project No. 16-38-60187).

Experimental modeling of lightning strike in sand soil

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Nowadays the protecting of power grid equipment against overvoltage caused by lightning strikes is important task, because on the one hand, the supplying of electricity without blackouts is critical issue, on the other hand, the usage of semiconductor control circuits in smart grids requires additional overvoltage protection. When lightning strikes in electric power facilities the resulting surge occurs and its amplitude depends on the properties of the grounding system, which are in dependence on the soil conductivity and the process of lightning current spreading in the soil are crucial in this regard. On the territory of the Russian Federation there are many sorts of soils with their properties, there are soils that have low conductivity (sandy, rocky, permafrost soils). Measurement of the properties at the field conditions, as well as the study of lightning current spreading process–an important issue in the design of grounding

systems. To conduct such studies mobile testing facility that allows to model in the field of lightning discharge current into the ground was made. Discharge current profile corresponds to properties of lightning strike current. The studies were conducted in the Moscow region on the territory of the sand pit. The measured grounding resistance value in the traditional way was 50 Ohm. When the impulse of current of lightning amplitude was applied to grounding device this resistance value reduced to 13 Ohm. In the experiments current and voltage waveforms, the magnetic field value at a distance of 10 m from the discharge gap were also recorded.

On the parameters of the diffused vacuum arc with cerium oxide hot cathode

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Diffused vacuum arc with consumable hot cathode is one of the most perspective plasma sources for the development of spent nuclear fuel (SNF) plasma reprocessing technology. In this paper studies of the discharge on cerium oxide cathode that was started in [1] are continued. Cerium oxide simulates evaporation and ionization processes of the uranium dioxide—the main component of the most common SNF nowadays. Current-voltage characteristic of the arc at currents from 20 to 120 A was registered. Cathode temperature changed from 2.1–2.4 kK. With the help of Langmuir probe electron temperature was measured and plasma density was evaluated within the interelectrode gap and above the anode. Plasma spectra were registered in the range of 0.4–0.9 μm. The data of cerium oxide thermionic characteristics were obtained.

The study was supported by the Russian Science Foundation (grant No. 14-29-00231).

The study of the plasma streams characteristics of the substances (lead and silver) simulating spent nuclear fuel components

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Conversion of a solid substance into the low-energy ($\approx$ 10 eV) plasma stream is a one of the priority tasks for the developing nowadays method of plasma separation [1,2]. It is necessary to ensure the plasma source operation in the presence of a longitudinal magnetic field (up to 2 kG), buffer rf (radiofrequency) plasma and gas pressure up to 10 mTorr. In this study, the evaporation was realized using induction crucible heating. Then the vapor was ionized by an electron beam. The variation of the thermocathode (LaB_6) temperature and the crucible heater power allowed to reach the cathode–anode potential difference of 10.5 V. The maximum current in the discharge gap was 13 A. The study of the silver (107.9 amu) and lead (207.2 amu) plasma streams parameters (concentration, ion and electron energy) and their spatial distributions depending on the magnetic field value and the potential difference was carried out. Spectral analysis of the plasma stream profile was carried out. The study was supported by a grant of the Russian Science Foundation (grant No. 14-29-00231).

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Helicon plasma generation for development of the plasma separation method

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One of the key problems of the development of the plasma separation method for spent nuclear fuel is the generation of buffer plasma with a density of $\sim 10^{12}$ cm^{-3} and single ionization [1] in a chamber with conductive walls of volume ~ 1 m^3 with an external magnetic field of ~ 1 kGs. In the majority of studies devoted to helicon sources a plasma generation was carried out in volumes with typical diameters of 10 cm limited by dielectric walls and according to [2] the question of high-density plasma (about 10^{12} cm^{-3}) creation in a large volume with a conducting walls requires additional researches.

In this paper spatial distributions of electron temperature and density have been obtained depending on the magnetic field intensity (0–1 kGs), plasma forming gas pressure (0.1–10 mTorr) and the power transmitted from the rf (radiofrequency) generator into plasma. At fixed buffer gas pressure (5.9 mTorr) a decrease of the electron temperature from 8 to 6 eV in the chamber center with magnetic field increase was found. Furthermore, it was found that at a fixed pressure the plasma density in the chamber center changes when the magnetic field is varied and has a maximum value of 8.2×10^{11} cm^{-3} at 320 Gs.

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Ion mass separation modeling inside a plasma separator

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The results have been obtained in a continuation of the work for ion trajectories calculation in crossed electric and magnetic fields [1] and also in a close alignment with the plasma separation study development [2]. The main task was to calculate trajectories of ions of the substance imitating spent nuclear fuel in order to find a feasible plasma separator configuration. The 3D modeling has been made with KARAT code in a single-particle approximation.

The calculations have been performed under the following conditions. Magnetic field is produced by 2 coils of wire, the characteristic field strength in an uniform area is 1.6 kG. Electric field is produced by several electrodes (axial ones, anode shell and capacitor sheets) with electric potential up to 500 V. The characteristic linear size of the cylindrical separator area is 100 cm. The characteristic size of injection region is 1 cm. Spatial position of the injection region is inside the separator. The injection direction is along magnetic lines. Injected particles are single-charged ions with energies from 0 to 20 eV with atomic masses $A = 150$ and 240. Wide spreading angle range was investigated.

As a result of simulation a feasible separator configuration was found. This configuration allows to achieve more than 10 cm spatial division distance for the separated ions and is fully compliant with and supplementary to the vacuum arc-based ion source research [3].

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The propagation of the electrical potential of the butt-end electrodes in the radiofrequency discharge plasma volume

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Currently, the question about propagation of the end face electrodes potential into a magnetized plasma of radiofrequency (rf) discharge is little-studied. For plasma separation method [1, 2], this problem is one of the crucial. This work is dedicated to the study of this problem. A longitudinal magnetic field was produced by the Helmholtz coils in the cylindrical vacuum chamber with a diameter of 85.6 cm and a length of 200 cm. Rf discharge operates at frequencies of 4.4–5.3 MHz. Rf power absorbed by the plasma was in range of 0.5–1 kW. At the end faces of the chamber electrodes were placed. The electrodes were biased negatively with respect to the ground. The following electrode geometries were investigated: circle-shaped with a diameter of 5.5 cm and a ring-shaped with inner diameter of 23.5 cm and outside 29.5 cm. Argon was used as working gas. The radial profiles of electron density and temperature were obtained by the method of double probe. The plasma potential in the center of the chamber and its radial profile depending on electrodes voltage were studied by the floating probe method. Also, the plasma potential dependence on the argon pressure in the vacuum chamber was studied. This work was supported by the Russian Science Foundation (grant No. 14-29-00231).

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Doping graphene by hydrogen at its synthesis in the plasma jet reactor

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In recent years, research is being conducted to develop hydrogen storage systems using nanoporous carbon materials such as carbon nanotubes and nanofibers, fullerenes [1]. As the scale of the use of these materials is largely limited by their relatively high cost, highly relevant is a research aimed at the development of new principles and methods of commercial production of carbon materials with given structure and porosity of cheap raw materials. It has previously been shown that graphene obtained in large quantities by using the dc plasma torch of power of 30 kW have developed mesoporous structure represented by pores with sizes less than 10 nm [2]. We have produced hydrogenated graphene structure (graphane) with a ratio of C:H of 4:1 at% using more powerful plasma torch up to 45 kW. The synthesis has been carried out in a reactor in the plasma jet using argon and helium at a pressure of 350–710 Torr. As the carbon source hydrocarbons (propane, butane, methane and acetylene) have been used. The resulting products have been investigated by electron microscopy, Raman spectroscopy, porosimetry, thermogravimetry and x-ray photoelectron spectroscopy. Element composition studies have been made by using express gravimetry.

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Spatial-temporal diagnostics of the "plasma jet–surface of heat resistant material" system

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Using an automated measuring complex the spatial and temporal changes in the parameters and composition of nitrogen plasma jet flowing out of the nozzle of the plasma torch [1] were studied using spectral methods, with a plasma temperature of 12–15 kK and acting on the sample of MPG-6 graphite. Due to the heating of the sample to temperatures of 2500–3000 K the influence of its sublimating material on the component composition of the plasma was established, and the temperature of the incoming plasma flow in the sample's surface region was calculated. An original method based on the analysis of movement of optical inhomogeneities in a laminar flow ($V < 1000$ m/s) plasma stream, was used to make estimates of the plasma jet velocity near the sample interaction zone. As a source of optical inhomogeneities an extent graphite rod of small diameter (much smaller than the jet diameter) was used, using a short electromagnetic actuator the graphite rod was injected into the stream in a transverse direction. The resulting optical inhomogeneities from the heated rod are picked up by plasma stream and due to the atomic and molecular composition of the inhomogeneities these inhomogeneities start to move with the plasma stream's velocities. Combined analysis of the results of a two-positioning video recording opens up the possibility of finding the fundamental spatial-temporal distributions of the plasma jets velocities, at medium and high pressures in the range of velocities from a few to thousands of m/s and temperatures of 3000–15000 K.

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The influence of ultrasound on the breakdown of transformer oil

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It is known that under the influence of ultrasonic waves (that are generated in the liquid dielectric because of electrical effects and mechanical vibrations of the electrical equipment) a medium disturbance occurs, leading to alternating high and low pressure areas, tear of the liquid and the formation of cavitation bubbles from the dielectric decomposition products or the gasses that are naturally dissolved in liquid [1]. It is also possible to use low-power microwaves for degassing of the liquids [2] this is relevant when, for example, oil-filled equipment's impermeability is broken and air penetrates it. The aim of the study was to investigate the effect of low-power ultrasonic radiation on the breakdown voltage of transformer oil. To tackle this problem an experimental setup was used that was previously designed for researches in breakdown of both pure liquid dielectrics and the gas–liquid two-phase mediums, described in detail in papers [3]. Studies have shown that when the transformer oil is exposed to the ultrasonic waves of low power more than 2 W/cm^2, at the initial time the breakdown voltage of the oil decreases relative to the clean oil due to degassing and occurrence of cavitation bubbles. The breakdown voltage increases nonlinearly with an increase in ultrasound application time. The experimental data indicate the possibility of using ultrasonic waves of low power for degassing transformer oil. This work was partially supported by a Russian Fund for Basic Research (grant No. 15-08-00395).

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Divergent duct plasma-spraying torch testing

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In this paper, we present the results of studies of electrophysical and thermal characteristics of low-temperature divergent duct [1, 2] plasma generator designed for thermal spraying wherein the sprayed powder can be supplied directly into arc column or attachment regions or into free plasma jet. Basing the arc voltage value at a given current and a heat flow [3] in water-cooled parts of the plasmatorch we determine current-voltage characteristics and efficiency. Current–voltage characteristics in the range $I > 200$ A appears to depend on the flowrate—when increasing it from 1 to 3 g/s a falling section of the VI-curve is replaced by a slow-growing one, indicating a change of arcing mode. We also report on the results of speed, temperature, and particle size measurements obtained by a novel diagnostic system, equipped with four high-speed infrared CCD-cameras focused on different zones of the plasma injector.
This work was partially supported by the Russian Foundation for Basic Research grant No. 16-08-00245.

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[3] Tyuftyaev A S 2013 *High Temp.* **51** 160–166

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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

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IPCP RAS — Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1,

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IPE RAS — Shmidt Institute of Physics of the Earth of the Russian Academy of Sciences, Bolshaya Gruzinskaya 10, Moscow 123242, Russia

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

IPP RAS — Timiryazev Institute of Plant Physiology of the Russian Academy of Sciences, Botanicheskaya 35, Moscow 127276, Russia

ISP SB RAS — Rzhanov Institute of Semiconductor Physics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 13, Novosibirsk 630090, Russia

ISPMS SB RAS — Institute of Strength Physics and Material Science of the Siberian Branch of the Russian Academy of Sciences, Akademicheskii 2/4, Tomsk 634021, Russia

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

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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, Tatarstan 420015, 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

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

MAI — Moscow Aviation Institute, Volokolamskoe Shosse 4, Moscow 125993, Russia

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

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NRNU MEPhI — National Research Nuclear University MEPhI

(Moscow Engineering Physics Institute), Kashirskoe Shosse 31, Moscow 115409, Russia

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

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

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

PNRPU — Perm National Research Polytechnic University, Komsomolsky Prospect 29, Perm 614990, Russia

PU — Princeton University, 40 Olden Street, MAE EQuad, Princeton, New Jersey 08544, United States

RSAU–TMAA — Russian State Agrarian University—Timiryazev Moscow Agricultural Academy, Timiryazevskaya 49, Moscow 127550, Russia

RSREU — Ryazan State Radio Engineering University, Gagarin Street 59/1, Ryazan 390005, Russia

SIM SB RAS — Sobolev Institute of Mathematics of the Siberian Branch of the Russian Academy of Sciences, Prospect Akademika Koptuga 4, Novosibirsk 630090, Russia

Skoltech — Skolkovo Institute of Science and Technology, Skolkovo Innovation Center Bldg 3, Moscow 143026, Russia

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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 RAS — Southern Scientific Center of the Russian Academy of Sciences, Chekhova Avenue 41, Rostov-on-Don 344006, Russia

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

STC UI RAS — Scientific and Technological Center of Unique Instrumentation of the Russian Academy of Sciences, Butlerova 15, Moscow 117342, Russia

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

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

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TUBAF, IIC — Institute of Inorganic Chemistry, Technical University Bergakademie Freiberg, Leipziger Strasse 29, Freiberg 09596, Germany

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