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The book consists of abstracts of plenary lectures, oral reports and posters presented at the XXXIV International Conference on Interaction of Intense Energy Fluxes with Matter (1–6 March 2019, Elbrus, Kabardino-Balkaria, Russia). The presentations deal with the contemporary investigations in the field of physics of extreme states of matter. The conference topics are as follows: 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; methods of mathematical modeling in physics of extreme states of matter; high-energy astrophysics; low-temperature plasma physics; physical issues of power engineering and technology aspects.

The conference is supported by the Russian Academy of Sciences.

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CONTENTS

Chapter 1. Power Interaction with Matter

Chapter 3. Equations of State for Matter

Chapter 4. Methods of Mathematical Modeling

Chapter 5. Physics of Low Temperature Plasma

1. Power Interaction with Matter

Thermodynamics of shock-wave and isentropic action on matter

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On the basis of general thermodynamic relations, the types of phase transitions available for realization in intense waves of adiabatic compression and expansion, as well as in powerful shock waves are discussed. The consideration is carried out in a general form, which assumes only the presence of local thermodynamic equilibrium in the system. The proposed formalism is used to study the dynamic methods of melting, high-temperature boiling and plasma phase transitions. Depending on the thermodynamic features of a substance, the thermodynamic conditions for the onset of shock discontinuity instabilities in a medium with an arbitrary equation of state are formulated.

This work is supported by the Presidium RAS within the fundamental research program "Condensed matter and plasma at high energy densities".

X-ray K and L terms estimation in free many-electron atoms and ions

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Information about x-ray K and L terms in atoms and ions is necessary for spectroscopic research method, astrophysical applications, calculation an ionization cross section of atoms and ions by other particles and so on.

The electron binding energies total analysis [1] has been applied to the K and L electron shells separately [2], and the atomic number Z scaling in atoms has been shown up. The simplest polynomial fit of the dependence made it possible to estimate the K, $L_{\rm I}$, $L_{\rm II}$, $L_{\rm III}$ x-ray terms in many-electron atoms with an error less than one percent and check a reliability of the experimental data.

In this paper, the method is extended to many-electron ions. The Dirac–Fock electron binding energy data $E_{nlj}(Z,z)$ (z is an ion charge; n and l are principal and orbital quantum numbers; $j = l \mp 1/2$) for some ions of the vanadium ($Z = 23$), palladium ($Z = 46$) [3] and uranium ($Z = 92$) [4] are used.

Polynomial fits of the functions $\log_{10}|e_n(\sigma_n)|$, $\log_{10} d_{nlj}(\sigma_n)$, $\sigma_n = \pi n Z^{-1/3}$ are applied to estimate K, $L_{\rm I}$, $L_{\rm II}$, $L_{\rm III}$ x-ray terms in some other ions of the same elements and ions of other ones. The error does not exceed 8%.

The method can be used for the new data verification, recovery the missing information about terms in any many-electron ion.

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Radial shear interferometer development for measurement the kJ-class lasers beams wavefront

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Nuclear fusion is one of the most promising and forwardlooking directions in search of new sources of energy. Inertial laser confinement theory was described in the seventies of the twentieth century; the spherical tritium-deuterium target is symmetrically illuminated by a many beams nanosecond laser. The existing concepts of inertial plasma confinement impose high extremely high requirements to the quality of laser beams which focused on a target or a resonators wall. To start a thermonuclear reaction, it is necessary to ensure uniform heating of the fuel mixture, which directly depends on the quality of the laser beams wavefront. The main causes of wavefront distortion in laser systems used in controlled thermonuclear fusion experiments are amplification, transport and focusing systems for laser radiation. Thus, in order to optimize the optical system, arises the problem of monitoring the shape of the laser pulse wave front at the output of the amplification system, individual optical assembly and in the targets plane. The authors have developed an optical scheme of a mobile radial-shear interferometer, which allows working with laser radiation at two wavelengths of 527 and 1054 nm. A laser attenuation system, consisting of a polarization beam splitter and a polarizer, was developed to match the energy level of the measured beam with the components damage threshold of the optical scheme. It allows to vary the amount of attenuation in the range of up to 10^{-4}. The interferometer is designed to measure wavefront distortions in a laser beam wavefront of 20×20 mm in size with an amplitude resolution of 20 nm with a spatial resolution of 20 μm.

Physical processes during laser ablation into a liquid and during laser shock-wave pinning

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The most important modern laser technologies include (i) the generation of colloid nanoparticles (NPs), laser ablation into a liquid and (ii) surface hardening of products by laser shock pinning. Significantly, with laser pinning, the surface to be treated is washed with water. Therefore, the physics of processes during ablation into a liquid and during pinning is common. True, the accents are different. If the ablation in the liquid actually forget about the shock wave (SW) generated by the impact, and leaving the thickness of the target, in the problem with pinning, on the contrary, the main question is about the impact. In addition, the role of water in (i) and (ii) is different. In (i) fluid contributes to the formation of NPs and adopts NPs, gently slowing them. Whereas in (ii) water is needed to enhance the recoil and increase the amplitude of the hydrocarbon in the product. The complete picture, developed in the work, of course, should include both edges: and the formation of ejection into the liquid as a result of ablation (i.e. (i)) and observation of the SW wave from the nucleation stage to its attenuation in the product volume (i.e. (ii)).

Electron-ion energy exchange in liquid aluminum within Ziman approach

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The coefficient of electron-ion energy exchange in a nonequilibrium two-temperature electron-ion system of a metal that occurs under the action of ultrashort laser pulses is an important kinetic coefficient, along with the coefficient of electronic heat conduction determining the dynamics of heating a target by a laser pulse. At the same time, the intensity of the laser pulses can be sufficient to melt a metal. An effective approach to calculating the electronic kinetic coefficients in the liquid state is Ziman approach, which uses the relaxation time approximation with allowance for the ionic structure factor for electron-ion scattering. Within this approach, it is possible to obtain both single-temperature and two-temperature (at unequal temperatures of electrons and ions) values of resistivity and electronic thermal conductivity of liquid metals. However, Ziman approach was not applied to the coefficient of electron-ion heat transfer. This paper shows that the Ziman approximation can also be used to calculate the energy exchange between electrons and ions in a liquid metal. We consider aluminum relating to so called simple metals, having only s- and p-electrons being excited under the action of laser irradiation.

Signatures of laser-induced silica glass densification in vibration and Raman spectra

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We perform a molecular dynamic simulation of vitreous silica irradiated by multiple laser pulses, and reveal an irreversible densification [1]. We calculate Raman spectra, and also perform partial and total vibrational analysis for glass models under investigation [2]. To reveal the structure of the vibrational spectrum, the characteristics of vibrational modes in different frequency ranges are investigated using a mode-projection approach at different symmetries. We consider the main experimental bands, and relate them to a detailed description of the vibrations. Finally, we compare our Raman and VDOS spectra with experimental measurements and apply a Sen-Thorpe analytical model to calculate an interbond angle. The relevance of the proposed research is due to the need for a quantitative description of the processes of change in the elastoplastic and optical properties of glass objects irradiated by laser beams.
We thank Presidium RAS Program No. 6 (Fortov V.E.) for financial support.

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[2] Shcheblanov N S, Povarnitsyn M E, Mishchik K N and Tanguy A 2018 *Phys. Rev. B* **97** 054106

Analysis of nanoparticles formation by ablation of Al under the action of femtosecond laser pulses into liquid water

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Nanoparticles of different sizes and water colloid mixtures of them can be produced as a result of femtosecond laser pulse action on a target in water surroundings. In order to generate the particles more effectively, it is necessary to understand the mechanisms underlying the laser ablation. For simulation of the laser pulse a continuum-atomistic model [1, 2] based on approach [3] is used. In this model the molecular dynamics is used for description of the ionic subsystem of metal while the electronic subsystem is described by the energy conservation equation solving. The model which is used represents all processes on the atomic level accurately including the nucleation processes in the metastabe liquid state and the dynamics of the formation of a liquid–gas mixture taking into account the effects of surface tension. The regimes of formation and destruction of aluminum nanoparticles of different sizes (5–100 nm) in water under the action of laser radiation of various intensities and frequencies are investigated.

We thank Presidium RAS Program No. 6 (Fortov V.E.) for financial support.

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Fragmentation of water droplet by ultra-short x-ray laser pulse

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We report about a numerical study of the fragmentation mechanisms of a micrometer-sized water droplet irradiated by ultra-short x-ray laser pulse. The results of the experiments [1, 2] show that the isochoric heating of such a droplet along the line of the laser beam lead to expansion of the droplet in the shape of a cylinder followed by its fragmentation. To unveil the underlying processes, we perform molecular dynamics (MD) simulations and simulations using the smoothed particle hydrodynamics (SPH) method [3]. Simulations demonstrate that a heated zone along the line of the laser beam generates a shock wave propagating from the axis to the rear side of the droplet. Fast expansion of the heated zone transfers the droplet to metastable state, as a result cavity is formed. Reflection of a shock wave from the rear side of the droplet produces a region of highly stretched material where spallation may occur depending on the laser pulse intensity. Comparison of MD simulations with results obtained from SPH demonstrates complete similarity between water droplets of different sizes.

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Atomistic simulation of laser ablation of silicon and crystallization of silicon nanoparticles

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Laser fabricated resonant nanoparticles (NPs) of silicon have been employed for a broad range of applications, namely, for directional and tunable light scattering, sensing, nonlinear light frequency conversion, optical heating with nanothermometry, and monitoring of thermally induced chemical reactions. It can be assumed that the mechanism of NPs formation in this work is similar to the laser ablation mechanism. So, the laser ablation process in the various conditions is studied using two-temperature atomistic model. The simulations are carried out in pseudo-1D atomistic case for laser ablation and the quasi-2D case for NPs crystallization. The ablation thresholds of surface ablation by ultrashort laser pulse of variable width τ_{las} at various temperatures of silicon are calculated. Also, the dependence of the modification depth d (ablation or melting) on absorbed fluence F is obtained. When the absorbed laser energy becomes higher than a particular threshold value, a liquid droplet of molten material is detached from the film surface. The formed droplets are cooled by collisions with air molecules during the movement from the irradiated film to the receiving substrate. The influence of cooling rate on NPs final state is studied due to unique optical properties depending on the atomic structure. As a result, the diagram of the silicon NP crystalline state just before the moment of contact with the receiving substrate is obtained using atomistic simulations and theoretical estimates.

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Electron-ion relaxation in Al nanoparticles: Non-adiabatic wave packet molecular dynamics

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Fast progress in nanoplasmonics determined strict requirements for the synthesis of nanoparticles with specified geometrical properties. Reshaping under femtosecond laser pulses has become a promising technique for such task [1]. Ultrashort laser impulses of high intensity excite electron subsystem which then transfers energy to ions via electron-ion relaxation and transforms the nanoparticle into so-called warm-dense matter state (WDM). WDM remains the subject of great scientific interest from both experimental and theoretical point of view.

Here by means of eFF potential [2] we apply non-adiabatic wave packet molecular dynamics (WPMD) approach to calculate the structural evolution of fs-laser irradiated aluminum nanoparticles during the first picoseconds after irradiation. The eFF potential provides the combination of particle dynamics for ions with wave packet dynamics representing electrons as floating Gaussians. eFF does not utilize Born-Oppenheimer approximation allowing us to model structural properties and non-adiabatic electron dynamics, such as electron-ion relaxation, within a single framework. Our results demonstrate a significant influence of the electronic pressure on the processes of thermalization, melting and acoustic vibrations launching in metal nanoparticles under fs-laser irradiation.

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Observation of relativistic laser pulse driven magnetic field in wire-shape Cu–Al target

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Strong magnetic fields of different configurations helps experimentalist to challenge many different physical problems like astrophysical phenomena, Internal Confinement Fusion and many others. In this work we observe magnetic field generation by the electron current driven by relativistic intensity ($\geqslant 10^{18}$ W/cm^2) short pulse (1.5 ps) laser. For this aims specially designed target, consist of 10 μm aluminum foil and long copper wire attached toward the rear side. After the laser irradiates the target, hot electrons propagate along the wire surface creating strong electric current, which generate magnetic field around the wire. To indirect conformation of the current inside the wire, copper x-ray spectra was observed using two focusing spectrometers with spatial resolution (FSSR). Resulting spectra shows strong K_α emission from the wire. This emission is created by hot electrons passing through it. Image of copper part of the target was obtained by Cu K_α imager. This image also shows heating of the wire by hot electrons.

Absolute intensities of x-rays radiated from solid-state targets irradiated by petawatt laser pulses

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Influence of different spectrometric equipment on a shape of x-ray spectra obtained for a wide (4.5–7.5 Å) wavelength range during interaction of high-intensity ($> 10^{21}$ W/cm^2) laser pulses with thin (2–20 μm) Si foils was investigated. As a result, the intensity of a plasma x-ray source formed in the laser focal spot was obtained in absolute units. It allows to check theoretical predictions from [1, 2], where it was shown that an experimental spectrum obtained for the same conditions can be fitted theoretically only after including in calculations the x-ray source with the intensity 10^{19} W/cm^2.
The work is supported by the Presidium RAS within the fundamental research program "Condensed matter and plasma at high energy densities".

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High energy density plasma generation with ultra-intense ($I \sim 10^{22}$ W/cm^2) femtosecond laser pulses

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Plasma formed by femtosecond laser pulses with ultra-relativistic intensities on thin solid-state foils is of great interest as bright source of various radiations. X-ray radiation diagnostic allows to provide the monitoring of plasma source parameters. This work we focused on studying features of x-ray emission from plasma generated by femtosecond laser pulses when its intensity on target surface reached ultra-relativistic value $I_{\text{laser}} \sim 10^{22}$ W/cm^2. We report about x-ray spectroscopy measurements done at recent experiments on J-KAREN-P laser facility and following plasma parameters determination. We shown the matters state with ultra-high energy density $\approx 8 \times 10^8$ J/cm^3 reached in the laser target interaction region.

Impurities utilization for x-ray measurements of parameters in recombining plasma

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Measurements of plasma are widely related with opacity issues when dense hot object is created by intense laser beams and expands in medium or vacuum. Usually targets irradiated by lasers have impurities, for example, oxygen layer on the front side. Very low amount of this material leads to completely optically thin plasma which makes it possible to use in researches by means of x-ray spectroscopy. This work aims the studying the astrophysically-relevant plasma created by laser with intensity around 10^{13} W/cm^2 and focal spot ≈ 600 μm on CF_2 (Teflon) target with impurity of oxygen at the ELFIE nanosecond laser facility (Ecole Polytechnique, France). Since plasma is in recombination mode far enough from target surface, the quasi-stationary approach was applied [1]. Relative intensities of transitions of a resonance series of oxygen H-like multicharged ions were used to determine parameters of the recombining plasma. It has been demonstrated that the intensities of the indicated transitions are sensitive to the plasma density in the range $N_e \sim 10^{16}$–10^{20} cm^{-3} at temperatures of 10–100 eV. The results were obtained by this method for all expansion range in experiment. The opacity analysis was conducted to demonstrate plasma to be optically thin.

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Properties of laser beam passed through cluster plasma studied with diffraction pattern method

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Knowledge of spatial, spectral and coherence properties of the laser radiation is of key importance for planning and interpretation high-energy-density physics experiments. In the frame this work we propose the diffraction method for determining such parameters of laser beam. So the spatial coherence and spectral composition were defined by analyzing the diffraction images formed during the passage of optical radiation 800 nm through cluster plasma and 200 μm Cu-wire. The propagating of radiation wavefront was simulated by using the software framework WavePropaGator (WPG) [1, 2]. The intensity distribution of laser radiation across beam was registered in the plane of LiF detector. Also the contribution of x-ray radiation generated from laser-cluster interaction into the observed diffraction pattern signal was found.

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Initial stages of plasma expansion of thin foil targets irradiated by high-power laser

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The study of the interaction of high-power laser beams with the matter is of great interest for more than half a century. One of the main issues here is the plasma density estimations in the interaction region because this cannot be done directly using traditional x-ray diagnostic methods because obtained emission spectra are usually space- and time-integrated ones. We propose an approach [1] that allows using spectral lines of H- and He-like multiply charged ions of such emission spectra of the laser plasma to estimate initial target parameters at the moment of laser pulse arriving. One can also evaluate additional information whether the target was destroyed by the laser prepulse and what was the quality of the laser contrast. The calculation was performed using an atomic kinetic code and was based on the idea of taking into account the relative "weights" of the various stages of plasma expansion. The results showed that it is not necessary to use non-stationary modelling in calculations. This also gave us information about the role and its influence on the integrated spectrum of the later stages and the type of plasma expansion. This method be used to analyse the results of experiments with so-called limited mass targets, for example, nanofoils or thin wires; and last but not least to evaluate laser contrast. As an example, specific calculations were made for aluminium and silicon plasmas. The work is supported by the Presidium RAS within the framework of the basic research program "Condensed matter and plasma at high energy densities".

[1] Martynenko A, Skobelev I and Pikuz S *Applied Physics B* **125**

Optimization of the hard x-rays yield from silver targets

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The hard x-ray radiation is used for radiography of a substance with the high energy density. A semi-analytical model for the generation of bremsstrahlung x-rays in metal targets, taking into account the refluxing of hot electrons, has been developed. The energy distribution function of hot electrons was determined by simulating measurements of bremsstrahlung and K_α radiation from silver targets that did not recirculate hot electrons generated by *s*-polarized subpicosecond laser pulses with intensity of 2×10^{19} W/cm^2 on the PHELIX laser system. Calculations of the x-ray bremsstrahlung yields in the energy ranges of 10–100 keV and 0.1–1 MeV, as well as the K_α radiation yield with a photon energy of 22.1 keV, from the front and back sides of silver targets of various thickness were carried out, taking into account, and without regard to the refluxing of hot electrons. It is shown that the effect of refluxing of hot electrons in thin foils leads to a significant increase in the yields of the K_α radiation and bremsstrahlung in the photon energy range of 10–100 keV. In contrast, the yield of bremsstrahlung photons in the range of 0.1–1 MeV from thin foils of 10–20 μm thickness in which hot electrons are recirculated corresponds approximately to the maximum yield of the photons from thick targets in which refluxing is insignificant. When using a silver foil with thickness of 10 μm, in which hot electrons are recirculated, the conversion efficiency of laser energy into bremsstrahlung energy in the range of 0.1–1 MeV is 4×10^{-4}. With such a value of this coefficient, it is possible to obtain radiographic images of lead samples of millimeter dimensions heated by a beam of heavy ions to states with high energy density. The prospect of obtaining by an order of magnitude greater conversion efficiency is indicated when using a layered target consisting of aluminum and silver foils, in which hot electrons are recirculated.

Laser-driven magneto-inertial fusion with magnetized cylindrical target

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A magneto-inertial (MIF) version of the thermonuclear scheme with a laser driver is considered in the work. This scheme is based on the general idea of adiabatic acceleration (compression) by a laser pulse of a target consisting of a pre-formed low-temperature plasma and a "frozen" magnetic field in the plasma. To study the physical and technical properties of the MIF scheme, a one-dimensional axisymmetric computational model is used in the active zone of a pulsed thermonuclear reactor. LD MIF assumed plasma and magnetic flux compression by quasisymmetric laser-driven implosion of magnetized target. We develop a 1D radiation MID code and a formulation for the one-fluid two-temperature equations for simulating compressible non-equilibrium magnetized target plasma. Laser system with pulse radiation with 10 ns duration is considered for numerical experiments. A numerical study of a scheme of magnetized laser-driven implosion in the external magnetic field is carried out. We have developed a model for LD MIF target implosion in an externally applied magnetic field. The main plasma parameters, magnetic field characteristics and laser radiation parameters along the radial coordinate are calculated. Numerical modeling of the laser target compression process showed the following. The central part of a target is optically transparent for both laser and own broadband plasma radiation during compression. However at the same time heat flow density on the first wall of the reactor chamber at a certain moment of time can reach 100 MW/cm^2. The magnetic pressure during compression of a target changes in time and is comparable to the static pressure Mbar. The maximum values of plasma pressure and temperature are observed after reflection of a shock wave from a geometrical axis of symmetry. This work is supported by the Russian Minobrnauki (project No. 13.5240.2017/8.9).

Laser–matter interaction modeling in relation to extreme-ultra-violet source development

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Modern extreme-ultra-violet (EUV) lithography requires a stable source of emission with high power and conversion efficiency in 2% spectral band near 13.5 nm. The most promising source of EUV radiation is based on hot tin (Sn) plasma, produced by a CO_2 or Nd:YAG laser. At first a distributed target is prepared using low intensity pre-pulse, then it is irradiated by main high intensity laser pulse thus producing the EUV-emitting tin plasma.

Numerical simulation of these processes is a non-trivial task. Complex self-consistent physical model is required. It should contain hydrodynamics (2D at least), radiation transport, thermal conduction, laser-matter interaction physics, two-phase equation of state and radiative properties.

The most interesting results related to simulation of laser impact on a tin droplet, subsequent target evolution and EUV-source radiation, as well as results of comparison with available experimental measurements of laser absorption and droplet velocity after laser pre-pulse [1], are presented in this report. Good agreement with experimental results has confirmed applicability of the considered model [1–3].

This work has been supported by the Russian Science Foundation (grant No. 14-11-00699). Calculations have been performed at high performance computer K-100 (KIAM RAS).

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THERMOS toolkit: Hollow ions simulations

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The THERMOS toolkit [2] has been used for simulation of plasma with presence of exotic ion states called hollow ions, which occur in high energy density experiments on modern XFEL facilities and can be used for plasma diagnostics. In order to simulate such plasma certain effects need to be taken into account, namely, the inner ion shells need to be emptied explicitly during atomic database calculation according to certain conditions [2]; ionization potential depression also need to be taken into account due to high density of matter; in some cases it is also necessary to utilize ionization and recombination crossections calculated with detailed atomic codes. This work has been supported by the Russian Foundation of Science (project No. 14-11-00699). Calculations have been performed at high performance computer MVS-10P (JSCC RAS).

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THERMOS toolkit: Solver for non-stationary system of rate equations

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Simulation of non-stationary processes taking place in plasma is a challenging problem. For a while it is been approached with various approximations, which have simplified the initial task to some extent providing the actual computability. Recent advances in high performance computing gradually gave researchers the capability of unreduced accounting of the non-stationarity effects in practical simulations. For instance, the latest NLTE10 workshop [1] offered to its participants a set of non-stationary tasks for aluminium and neon plasmas, based on recent experiments performed at XFEL facilities. In order to gain the capability of modeling non-stationary problems a new module has been developed and introduced into the THERMOS toolkit [2]—a highly efficient solver for non-stationary system of rate equations. This work has been supported by the Russian Science Foundation (project No. 14-11-00699). Calculations have been performed at high performance computer MVS-10P (JSCC RAS).

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Excitation of spins in iron borate by intense THz pulse

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Ultrafast control of the order parameter (the electric polarization or the magnetization) in ferroics is a topical problem, the solution of which is important for the progress in information technologies. In this regard, the use of electromagnetic radiation to change the state of the order parameter is of considerable interest, as it allows to overcome the problems inherent in modern electronics, such as, for example, energy dissipation due to ohmic losses. In recent decades, substantial progress has been made in the field of ultrafast optical control of spins in ferromagnets and fully optical magnetic recording. Recently, ultrafast coherent control of magnetic phase transitions has been demonstrated by active optical pumping of a soft mode [1] and reversal through a strongly nonequilibrium state [2]. The latest advances in the development of strong THz sources have opened a doorway for coherent control over magnetism at ultrashort time scales [3]. Here we demonstrate that a strong nearly single-cycle THz pulses with amplitude of up to 0.5 MV/cm (0.2 Tesla) excite the quasi-antiferromagnetic (q-AFM) mode in a weak ferromagnet iron borate ($FeBO_3$). The amplitude of the q-AFM mode scales linearly with the strength of the THz magnetic field as expected for the excitation by the magnetic field torque.

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Towards high-intensity THz pulse generation in two color filaments of terawatt laser radiation

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Terahertz (THz) pulses with electric field power above MW/cm are now requested for strong field applications lice: particles acceleration, short electron bunches measurements, controlling the state of matter [1]. The advantage of a THz pulse in comparison with the visible frequency range one—in the quasi-stationary, non-oscillating field direction, with a ps duration, the interaction with particles or ions accumulates by orders of magnitude more efficiently. The only way to get THz pulses of MV/cm intensity is the conversion of high-power fs laser pulses. Preliminary experimental results are analyzed in several ways of generating THz pulses (optical breakdown plasma, non-linear crystals) from the radiation of the Pulsar-200 TW laser subpetawatt laser system, operating at NRC "Kurchatov Institute" and also from the mJ laser system at MSU. Both laser systems are based on TiSa media. The prospects for scaling the generation of THz to the Joule laser pulses energy are discussed.

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Intense THz induced second harmonic generation from $Ba_{0.8}Sr_{0.2}TiO_3$–MgO structure

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The ability to switch ferroelectric polarization between two ground states by electric field of THz pulse is perspective method to ultrafast control of order parameter.

Recently it has been realized that experiments in which dynamics of the ferroelectric order parameter is triggered with an intense THz pulse and probed with the help of second harmonic generation is a powerful tool in fundamental studies of ultrafast dynamics in ferroics [1, 2].

In our experiments we have excited the $Ba_{0.8}Sr_{0.2}TiO_3$–MgO using intense nearly single-cycle THz pulses with the electric field up to 1 MV/cm. Although the observations can be mistakenly interpreted as oscillations of the electric polarization at the frequency of the soft mode and switching of the order parameter to another metastable state, here we show that the THz modulation of second harmonic generation in structure has a purely optical origin.

In particular, we have shown that dynamics of the non-linear signal must be explained in terms of the interference of the static and relativistically moving sources of the second harmonic generation.

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Laser engineering of the surface of GdFeCo–IrMn structures

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The family of GdFeCo alloys, which are basis of the optical recording medias, has been manifested new application for super fast memory devices based on non thermal all optical magnetization reversal initiated by polarized light of femtosecond laser [1]. In the irradiated area the critical field of the magnetization reversal remains practically same, but additional good reproducible feature of the magnetization reversal takes place in non irradiated areas. The switching of magnetization starts in slightly smaller fields in comparison with irradiated areas. Amplitude of the magneto-optic Kerr effect signal decreased down top 1.7 times correspondently to local thinning of the laser irradiated area. Laser engineering of the surface of GdFeCo thin films opens new opportunities for local control of energy balance between magnetic anisotropy, exchange interaction and Zeeman energy. This can be used to create individual separated sectors on the surface of the magnetic films for capture, storage and analysis of the ferromagnetic nanoparticles and magnetically labeled biology cells [2].

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All-optical magnetization switching in amorphous ferrimagnetic rare-earth transition-metal alloy DyFeCo by femtosecond laser pulses

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Since the fundamental limit of the application of ultrashort strong magnetic field pulses to switch the magnetic order in the medium was shown in 2004 [1], researchers trying to find new approaches to magnetic recording technologies.

One of such approaches, the switching of the magnetic state of the medium by femtosecond laser pulses, was first demonstrated in 2007 in a ferrimagnetic alloy of rare-earth metal and transition metal [2]. This phenomenon was found in a different class of materials [3], but the mechanisms responsible for all-optical switching are not always clear.

In our study, we investigated the local all-optical switching of the magnetic order in a thin film of amorphous ferrimagnetic rare-earth transition-metal alloy DyFeCo by femtosecond laser pulses, as well as the magnetic properties of this material.

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The temperature dependence of the photoinduced soft mode in $Sn_2P_2S_6$

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The modern micro- and nanoelectronics development is expressed in the ever-growing demand for information recording speed increasing. In traditional memory devices the recording information speed is determined by the magnetization switching speed. In [1], the possibility of magnetic order parameter switching under the single femtosecond laser pulse action was demonstrated. At present it is the most effective way control the medium at extremely short times. Application of the same technique to ferroelectric materials will allow to build new effective and non-volatile memory devices. However, the problem of ultrafast ferroelectric order parameter switching is not solved yet. The reason is there are no the same mechanisms in ferroelectric materials, which provide the ultrafast magnetization switching in magnetically ordered media.

Earlier we demonstrated the possibility of ferroelectric soft mode optical excitation in the ferroelectric-semiconductor crystal $Sn_2P_2S_6$ [2].

Here we present the results of the temperature dependence studies of the photoinduced soft mode in the $Sn_2P_2S_6$ crystal. We show that its behavior reminds the soft mode one near the phase transition. However, the observed decrease in the oscillation frequency in the vicinity of Curie temperature T_c is much weaker than previously reported. This can be explained by the shadowing of the pure soft mode by its interaction with other photoinduced modes.

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High-power femtosecond radiation for THz semiconductor antennas

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Epitaxial InGaAs films are promising material for creating photoconductive antennas for the generation of THz radiation. The main disadvantage of such films is the low resistivity. This leads to a high dark current and high breakdown voltage. To increase the resistivity, different approaches are used: fabrication of the superlattices [1], iron implantation [2], epitaxial growth in low-temperature mode with doping with beryllium atoms [3], etc. Another problem of THz antennas is their fragility, damage and large losses in the optical-terahertz transformation. In order to increase optical-to-terahertz conversion passivation layers are using (SiO_2 and Si_3N_4) [4]. The molecular beam epitaxy method was used to create two samples with a functional layer superlattice $In_{0.53}Ga_{0.47}As$–$In_{0.52}Al_{0.48}As$. A passivating dielectric Si_3N_4 was applied on the surface of one of the samples. Terahertz time-domain spectroscopy was used to study the efficiency of the generation of THz radiation. It was experimentally shown that the intensity of THz radiation from a functional film with a dielectric is two times greater than that from a similar film with the same optical pump power. The dependence of the THz radiation intensity on the optical fluence on a film with a dielectric reaches a saturation level with values of 398 $\mu J/cm^2$. At the same fluence on the film without a layer of Si_3N_4, the destruction of the film surface was observed.

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Photoexcitation carrier kinetics in transition metal dichalcogenides

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To investigate the optical properties and carrier dynamics of transition metal dichalcogenides (TMDs) as well as the relaxation time for hot photocarriers in TMD monolayers, the two-color pump-probe experiment was performed at room temperature.

The model was proposed which takes into account the difference between the exciton regime and the electron-hole plasma regime. In the first case the Coulomb interaction between electrons and holes and the presence of exciton resonances plays the most important role in the behavior of optical parameters. In the second case (with a high carrier density), screening and other effects play the most important role: plasma contributions of free electrons, renormalization of the band gap, and band filling. These effects alter the optical properties of the material, including the refractive index. A change in the spectral dependences of the optical parameters with a change in the carrier concentration allows us to calculate the dependence of the reflectance on the carrier concentration. The spectral dependences of real and imaginary parts of refractive index for unexcited sample for different number of layers via the change of the band gap as well as other parameters of the resonances are also taken into account. Numerical calculation of the reflectivity dependence on carrier concentration together with the calculation of the time dependence of carrier concentration allows to simulate time dependence of reflectivity.

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Impact of strong picosecond THz pulses on dielectrics

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Direct manipulation of the atomic lattice using high power single-period THz pulses allows to create new states of matter in complex materials. This is possible due to strong anharmonicity of ionic potential due to excitation by strong transient electric field of THz pulse, which ranges up to tens of MV/cm. This pulse can dynamically alter the lattice structure and provide through phonon-phonon coupling coherent control over specific phonons including soft modes. Two types of unharmonic processes were reported so far. The first one is to resonantly excite high frequency vibrational mode and to modify the lattice structure through indirect coupling of this infrared-active phonon to other, lower frequency lattice modulations [1]. The second one is opposite: to drive the lowest frequency optical phonon in the into the anharmonic regime with a strong terahertz pulse and transfer energy to higher frequency phonon modes through nonlinear coupling.

In this paper, we utilize optical pump probe scheme in which THz pulse is used as a pump, and a femtosecond optical pulse is used as a probe. For detection, the second harmonic of the optical pulse generated in ferroelectric crystals is used as a measure of structural changes. Additionally to phonon spectra, which demonstrate up-conversion, THz power dependences of different spectral components are measured. The latter shows non-trivial dependences which points to structural changes as well. The work is supported by Ministry of Science and High Education via state tasks 16.4699.2017/6.7 and 3.1923.2017/4.6.

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Generation of terahertz radiation under laser action on hot dense plasma

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The generation of terahertz (THz) waves in the interaction of a femtosecond laser pulse with hot dense plasma by using the Vlasov kinetic equation has been studied. The penetration of laser radiation into the plasma in the regime of anomalous skin effect has been considered. Excitation of low-frequency fields in the skin layer of a dense plasma under laser action has been studied. It is shown that, in the case of a femtosecond laser pulse, these fields can be emitted into vacuum in the form of THz waves. Analysis of the frequency characteristics of the generated THz radiation has shown that, for a tightly focused laser pulse, the spectrum has a wide peak near the frequency, which is comparable with the reciprocal laser pulse duration. It is shown that an increase in the focal spot size leads to a shift of this spectral line toward lower frequencies and a decrease in the height of the spectral peak. The directional pattern of THz radiation has been studied as a function of the tightness of laser focusing. It is shown that, for a tightly focused laser pulse, the THz radiation is pressed to the plasma surface. An increase in the focal spot size leads to an increase in the propagation angle of THz radiation with respect to the plasma boundary. If the transverse size of the laser pulse is sufficiently large, THz waves are emitted almost normally to the plasma boundary. The total energy of the THz pulse has been calculated. It is found that, for fixed values of the energy and duration of the laser pulse, the total energy of THz radiation is maximal in the case of tight focusing. It is established that the total energy of the THz signal is independent of the plasma density and proportional to the square of the electron temperature.

Secondary sources of super-ponderomotive electrons and hard radiation in relativistic laser–matter interactions

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We present our theoretical analysis of experimental results on interaction of relativistic sub-picosecond laser pulses of PHELIX system with sub-mm long near critical density (NCD) plasmas. The effect of the relativistic laser pulse channeling and creation of quasi-static azimuthal magnetic and radial electric fields that keeps electrons in the channel ensured effective coupling of the laser energy into energetic electrons. Application of sub-mm thick low density foam layers provided substantial increase of the electron acceleration path in a NCD-plasma compared to the case of freely expanding plasmas created in the interaction of the laser pulse with solid foils.
Both measurements and 3D-PIC simulations show high directionality of the acceleration process, since the strongest increase in the electron energy, charge and corresponding gamma-yield was observed close to the direction of the laser pulse propagation. Obtained results of simulations are in a good agreement with measurements and indicate the effective electron acceleration in NCD plasmas with a total charge of electrons about 2 μC at the energies above ponderomotive one ($E > 3$ MeV). The charge of super-ponderomotive electrons that are suitable for direct radiographic applications with $E > 30$ MeV reaches a very high value of 80 nC.

Preservation of the electron beam polarization and emittance in the laser plasma accelerator

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Laser-plasma acceleration is a promising method, alternative to traditional radio frequency accelerators, whose relatively small acceleration gradients lead to their large size and considerable cost. However, in order the beams of ultrarelativistic particles accelerated using this method will be suitable for practical applications and experiments in high-energy physics, they need to be of high quality with preservation of the initial polarization and small emittance, angular divergence and energy spread. In this work, we focused on the study of the dynamics of the electron beam emittance and polarization in nonlinear and non-constant fields generated by a short relativistically intense laser pulse in a plasma channel. Using the developed model [1], numerical calculations and theoretical analysis of the emittance growth under the action of a nonlinear focusing force in the process of laser wakefield acceleration were carried out. The effect of matching the initial emittance of a beam with a focusing force on its final value was shown. It was demonstrated that the dynamics of the emittance affects the process of electron depolarization. In our work, we took into account the effect of synchrotron radiation of electrons on their characteristics and also studied the contribution of quantum effects associated with the radiation to the final depolarization of a particle beam. This work was supported by the Russian Foundation for Basic Research (project No. 19-02-00908/19).

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Electron acceleration in foams under various laser focusing conditions

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The objective of this work is a numerical study of the acceleration of electrons from near-critical targets of submillimeter size under the action of a petawatt laser pulse. The pulse parameters used in the simulation correspond to the real parameters that are planned to be used in the future experiments. The energy contained in the spot is 30 J. The duration of the laser pulse equals 750 fs. The laser spot is elliptical with major and minor axes equal to 6 and 4 μm, respectively. Such small spot is shown to be the favorable for electron acceleration in the number and energy of particles comparing to larger spots. The focusing point in the experiments can float. Therefore we study the influence of focusing point on the electron acceleration process. It can be placed before the target, at its surface and inside the target in the simulations. In addition, various mathematical approximations of the laser pulse are considered.

Acceleration of electrons in the interaction of subterawatt laser pulse with inhomogeneous plasma

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In this work, the influence of nonlinear phenomena of self-focusing and self-modulation of a laser pulse on the acceleration of electrons during the interaction of a femtosecond laser pulse of sub-gravity power with a gas jet plasma is considered. The three-dimensional modeling of the interaction of laser radiation with low-density inhomogeneous plasma by "particles in a cell" (3D PIC) showed that the self-focusing of the laser pulse, which occurs under conditions when its power exceeds the critical for relativistic self-focusing determined by the local density of plasma electrons, leads to effective generation of the plasma wave. Due to the effect of reducing the phase velocity of the wake plasma wave generated in the regime of self-modulation of the laser pulse, there is a capture of electrons into the accelerating phase of the plasma wave, and acceleration to energies of order 10 MeV. It is demonstrated that under the conditions of limitation of the electron acceleration region by the length of their dephasing, quasi-energy electron bunches with a characteristic energy of about 9 MeV can be formed. The effective temperature of the accelerated electrons and their angular distribution obtained in 3D PIC-modeling are in good agreement with the experiment.

Physical mechanism of electron bunch generation by an ultrarelativistic-intensity laser pulse passing through a sharp plasma boundary

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The physical mechanism of electron-bunches generation at the interaction of a laser pulse of ultrarelativistic intensity with semi-bounded plasma having a sharp boundary is studied in the one-dimensional geometry [1]. It is shown that electron bunches are generated by the laser pulse due to the multiflow motion of plasma electrons with crossing trajectories. It is revealed that the total charge of the electron bunch is formed of two different groups of electrons. One group consists of electrons that do not cross the boundary of ion background in the process of their motion. The mechanism of their accumulation in the bunch generated by the laser pulse implies that the self-injection of every electron from this group into the wake wave occurs at the time moment and space point, where the earlier injected electrons composing the bunch already are. The electrons of the other group cross the plasma ion background boundary and return. The mechanism of their accumulation into the bunch is such that after the return into the region of ion background these electrons move with greater velocities and overtake the bunch. An analytical relation that allows an electron bunch charge to be estimated as a function of plasma characteristics and electron trajectory parameters is derived and confirmed by the results of numerical simulations.

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New schemes for stochastic electron heating in laser plasma interactions

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A typical situation at the interaction of ultrashort relativistically strong laser pulses with plasma is presence of suprathermal particles in electron and ion distributions. In this report, we consider two schemes of for stochastic electron heating in laser plasma interactions. The first scheme exploits the scenario where a high contrast as well as a sharp plasma-vacuum boundary create unique conditions for the development of stochasticity in complex fields which are a combination of incident and reflected pulses, and possibly quasistationary fields, induced near the plasma-vacuum interface. Another scheme of stochastic instability development is electron acceleration and heating in cluster plasma when electrons are accelerated in combined fields of a laser wave and Coulomb field of a cluster. Our theorectial model predicts the enhanced electron heating for both schemes due to synergetic effects in complex laser and Coulomb fields and demonstrate that stochastic heating process may contribute to generation of suprathermal particles. The work was partially supported by the Russian Science Foundation (grant No. 14-12-00194).

Multielectron effects in secondary radiation generation during the interaction of atomic gases with intense laser pulses

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The present paper is devoted to the *ab initio* numerical simulation of the evolution of multielectron atoms and excitation of electron currents during gas ionization with an intense laser field. We develop computer code for numerical simulation of these processes on the basis of the time-dependent Kohn–Sham equations. Based on the performed calculations we show the importance of taking into account of multielectron effects during the calculation of electron currents responsible for generation of secondary radiation in terahertz, mid-ir, xuv and soft x-ray ranges. For sufficiently large number of electrons in the outer shell of an atom, the action of an external electric field leads to a significant polarization of the outer shell. This polarization creates a screening of the external field and leads to a decrease in the probability of tunneling ionization of atoms and an increase in the number of neutral atoms participating in the generation of secondary radiation. At large peak intensities of laser pulses, this corresponds to a significant increase in the power of secondary radiation in comparison with the case when the joint dynamics of many electrons on the outer shell is not taken into account. This work was supported by the Russian Science Foundation, grant No. 17-12-01574.

About linear impact of inductive accelerator high intensity electron beam on a tantalum target

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Linear inductive accelerator (LIA) is a good machine to obtain the small sized hard x-rays source. Intense electron beam is strongly focused to the LIA high Z target, e.g., tantalum target. Because of beam-target interaction, the target material, including impurities, goes through fast phase transitions and starts to affect the electron beam. This effect is observed during both the first pulse and the second pulse of LIA.

In this paper, it is shown that vaporized target impurities are the main reason of electron beam defocusing and the increase of focal spot sizes during the first LIA pulse. To research this process more carefully chemical and structural analysis of the target was carried out. It was obtained that the target melting caused by LIA pre-pulse minimizes defocusing effect.

In two-pulse mode significant increase of focal spot sizes was observed. Linear focal spot sizes–time-delay dependence was shown. This fact tells that electron beam defocusing can be caused by target plasma formation and its moving towards the second electron beam of LIA.

Effect of radiation hardening of optical fibers with unalloyed SiO_2 core and optical fibers production with record high resistance to pulsed ionizing radiation exposure

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It has been recently determined that self-trapped holes (STH) belong to two different types: proper STH and deformation ones. The proper STH appear on the weakly strained sections of the grass grid (with a normal or slightly decreased network length Si–O); the deformation STH appear on the strongly strained sections (with highly decreased network length Si–O). The results of this paper confirm that the effect of radiation-induced attenuation (RIA) decreasing in the optical fibers with an unalloyed SiO_2 core is evident because of its preliminary γ-radiation by a small dose of 100 Gy. So, the proper STH do not appear at the next pulsed radiations of optical fibers. This effect allows improving the radiation resistance of optical fibers even at non-optimized technology of preforms synthesis of unalloyed optical fibers with a shell made of fluorine-silicate glass. It was determined that the optimized unalloyed optical fibers illustrate a record low RIA at the pulsed influence of ionizing radiation, lower RIA than other types of solid optical fibers do including optical fibers alloyed by nitrogen, phosphorus that were earlier considered as the most resistant to the pulsed influence of ionizing radiation.

Photon equilibrium distribution in a fully ionized weakly interacted plasma

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The photon equilibrium distribution function is found for the systems containing a dense fully ionized plasma. It is shown that this distribution possesses a long tail for asymptotically large values of the photon momentum.

Comparison of laser breakdown and laser ablation ignition thresholds of combustible gas mixtures

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Laser ignition of fuel mixtures is now thoroughly studied for reciprocal, rotary, and jet engines as a substitution for traditional ignition systems providing higher reliability, broadening operation pressure range, available to ignite fuel lean mixtures with the relevant decrease in fuel consumption and harmful emissions. Evaluation of minimum laser ignition energies has shown that significant part of energy is not absorbed by gas, so just wasted.

Laser spark plug size and cost depend significantly on output pulse energy, so the most efficient use of the latter is desired. This can be implemented in laser ablation ignition. However, combustion core spoiling by the ablator and its lifetime are important issues to consider.

As almost no comparable data on gas breakdown and ablation ignition thresholds are published, we have performed an experimental investigation of minimum laser pulse energies at different ablator materials (Ti, Zr, SS304), fuel mixture (butane based) compositions ($\phi \sim 0.5$–1.3) and pressures ($p \sim 1$–3 bar).

The results show that laser pulse energy for fuel lean mixtures can be significantly reduced using the ablator, and leaner mixtures could be ignited at all.

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

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In this work, the action of laser pulses (thermomechanical ablation) with a duration 80 fs at a wavelength of 1240 nm on crystals of potassium chloride was studied [1, 2]. The experiments were carried out at the Center for Collective Use of Unique Scientific Equipment "Laser Femtosecond Complex" at the Joint Institute for High Temperatures of the Russian Academy of Sciences, on the terawatt femtosecond chromium–forsterite laser system [3].

Using an image processing program, the geometric dimensions R_x and R_y (lengths of the principal axes) of the damage spots were determined; they took the form of an ellipse due to the oblique incidence of the radiation on the target. It has been discovered that a linear dependence of the optical damage spot area (S) in the laser pulse energy (G) is higher than the crystal damage threshold: $S = K \ln(G/G_0)$, where G_0 is the energy of the optical damage and K is constant. For potassium chloride, $G_0 = 160$ μJ, and $K = 4440$ μm^2.

This work was supported within the framework of the basic part of the Government Contract of the Russian Ministry of Education and Science for Kabardino-Balkar State University for 2017–2019 (project No. 3.8382.2017/BCh).

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Investigation of the sodium chloride surface elemental composition after ultra short laser pulses effects

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The effect of laser radiation (40-fs pulses at a wavelength of 800 nm) on the surface of an ionic crystal were carried out on the terawatt titanium-sapphire femtosecond laser system included in the Center for Collective Use of Unique Scientific Equipment "Laser Femtosecond Complex" in the Joint Institute for High Temperatures of the Russian Academy of Sciences [1]. The power density in processing spot reached 90 TW/cm^2 [2]. The effects of laser irradiation were analyzed with the use of an x-ray photoelectron spectrometer (XPS) "Thermo Scientific K-Alpha". The elemental composition of the surface in the laser damage spot was studied. A comparative analysis of XPS spectra showed that sodium chloride has reduced oxygen content in the damage spot; in addition to changes in the phase state, there is a change in the medium at the molecular level. This work was supported within the framework of the basic part of the Government Contract of the Russian Ministry of Education and Science for Kabardino-Balkar State University for 2017–2019 (project No. 3.8382.2017/BCh).

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Laser ablation of the glass composites with transition metals

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The material destruction processes as a result of laser ablation are probabilistic in its nature [1–3]. This is due to the absorbing defects random spatial distribution and to the laser radiation characteristics random distribution. All of this lead to the different values of the laser breakdown threshold of the material surface and to the probabilistic nature of the laser plasma formation. Earlier, the authors of [2–4] carried out the experimental studies of the threshold energy densities at the pulsed laser ablation of the various materials, including composite materials based on silicate glass alloyed with transition metals (Au, Cu) under the action of a YAG-Nd laser radiation at a wavelength of 1.064 μm. The laser ablation destruction of the samples the threshold energy density resulting values allow to obtain its dependence on the composition, the composites optical and mechanical properties.

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Specific features of experiments with thick targets in the field of accelerator-driven system research at the Joint Institute for Nuclear Research

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The experiments are performed at two basic facilities of the Joint Institute for Nuclear Research: accelerator complex Nuclotron-M and phasotron. Nuclotron-M provides experiments at extracted proton and light ion beams in an energy range from 0.35 to 5 GeV/nucleon. Phasotron provides high intensity proton beams with an energy of 660 MeV. Specific features of experimental methods with thick targets are considered. Different applied methods are discussed: ionization method, track method, neutron detection, fission cameras, semiconductor detectors, etc. Various methods for monitoring and diagnostics of extracted beams required for experiments are presented.

New concept of accelerator-driven system power production with light ions

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Energy efficiency of proton and light ion beams for the accelerator-driven system power production is analyzed with account of accelerator type. It is shown that for light ions, beginning with ^{7}Li with energies > 1 GeV/nucleon, ion beams are more efficient than the proton beam with an energy of 1–3 GeV. The possibility of obtaining energy release in a quasi-infinite uranium target equivalent to that of 1 GeV proton beam with higher efficiency (and smaller accelerator size) is substantiated. The effects of the target size and converter material are studied.

Mach wave configurations generated by intense heavy ion beam as a scheme for investigation extreme states of matter

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To study high energy density matter in extreme state created by intense heavy ion beam schemes LAPLAS and HIHEX were proposed earlier [1]. The scheme proposed here is based on generation of Mach configurations of shock waves in targets by intense heavy ion beam. The advantages of the scheme are:effective utilization of the beam power (energy deposition in Bregg peak location is used); an existence behind Mach wave of matter region with practically 1D hydrodynamic movement suitable for experimental research.

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Effect of irradiation on the structural and electrical properties of $AgGe_{1.6}As_{0.4}(S+CNT)_3$ glassy composite material

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The effect of charged particles beam (protons and deuterons) on the electrical and structural properties of the $AgGe_{1.6}As_{0.4}(S+CNT)_3$ glassy composite material containing carbon nanotubes is studied. This material has a high share of ionic conductivity component, which is as less as 99% of the total conductivity at room temperature.

In this work, it was shown that after irradiation with a deuteron or proton beam, no significant changes in the magnitude and share of the ionic conductivity component are observed. However, there are changes in the magnitude of the electronic component of conductivity depending on the irradiation parameters which may be a consequence of structural reordering in the glass matrix of irradiation-modified material.

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Features of determination of the characteristics of the carbon plastic under pulse action

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Wide technological applications of the carbon fiber based composites cause the interest to their properties under pulse loading. It is typical e.g. at lightning strike. Complex of acting factors determining the material behavior includes, in particular, its reaction on a mechanical loading of characteristic duration. The results of the experimental study of carbon fiber based composite specimens, loaded at mode 1 with pulse magnetic impact of microsecond duration [1], are presented. The analysis of the data obtained using approaches described at [2] allowed to determine the characteristic parameter–energy accumulation time, determining the destruction process at dynamic loading. For the composite with filaments orientation $\pm 45^\circ$ in respect to tensile stress, the destruction process has threshold character. The energy of formation of new surfaces is determined, which appeared close to surface energy of destruction of igneous rocks.

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Explosive character of instability development for the free surface of a conducting liquid in an electric field

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The traditional approach to describing the dynamics of the free surface of a liquid in an external electric field is based on the use of perturbation theory in a small parameter, namely, in the amplitude of the boundary perturbation [1,2]. There remains an open question concerning the influence of the high-order nonlinearities, which are not taken into account in this approach.

In the present work, we show that the analysis of the potential energy functional for a conducting liquid allows us to make a number of non-trivial conclusions concerning the system behavior. For a symmetric spatially localized perturbation of the surface, which is directed upwards, it is proved that the part of the functional responsible for nonlinear interactions is negatively defined. Thus the nonlinearity plays a destabilizing role accelerating the development of instability and defining its explosive character. It is important that this result is obtained without restrictions on the amplitude of the boundary perturbations, i.e., it takes into account high-order nonlinearities.

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Nonlinear conditions for instability of the free surface of a conducting liquid in an external electric field in a confined axisymmetric geometry

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It is known that the free surface of a conducting liquid exposed to a sufficiently strong electric field is unstable [1]. For an unbounded free surface, the dynamics of instability development is defined by a nonlinear interaction of three plane waves that form a hexagonal structure [2].
In this paper, we consider the case of bounded axisymmetric system geometry. Given the influence of quadratic nonlinearities within the framework of the Hamiltonian formalism, we derive an amplitude equation that describes the evolution of the boundary. Using this equation, we find the condition for hard excitation of boundary instability, which leads to explosive growth of surface disturbances. The differences in the description of the dynamics of axisymmetric perturbations of the boundary from the cases of plane, square, and hexagonal symmetries of the problem are discussed.
The work was performed in the framework of state program 0389-2015-0023 and supported in part by the Presidium RAS (program No. 11), the Presidium UB RAS (project No. 18-2-2-15), and the Russian Foundation for Basic Research (projects No. 17-08-00430 and 19-08-00098).

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Prebreakdown processes in a metal surface microprotrusion exposed to rf radiation

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The vacuum breakdown that may occur at the walls of the accelerating structure of a TeV linear electron-positron collider exposed to rf electromagnetic fields is a major factor limiting the accelerating field strength [1]. Mesyats [2] proposed an explosive emission mechanism of the vacuum breakdown between electrodes subject to the action of microwave fields. According to this mechanism, the breakdown occurs due to the heating of microprotrusions by the emission current during the negative half-wave of the cathode voltage. In this work a two-dimensional two-temperature model has been developed to simulate the heating of a microprotrusion on a metal surface exposed to rf radiation of frequency 10 GHz. The numerical simulation using this model includes a self-consistent calculation of the electric field at the microprotrusion surface and the field emission characteristics of the microprotrusion using the particle-in-cell method, a calculation of the current density distribution in the microprotrusion, and a calculation of the lattice and electron temperatures with the use of the heat equation taking into account the Joule effect and the (finite) rate of the heat exchange between the electrons and the lattice. The microprotrusion heating time has been calculated in relation to the electric field enhancement factor and the electron-phonon interaction parameters.

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Study of spectral properties of the thin-film coated surfaces based on integral measurements

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One of the ways to control radiation heat exchange is to apply coatings on the surface that change the optical properties of the surface. The task of measuring the spectral properties of materials with applied thin-film coatings is particularly relevant today. Such coatings (for example, titanium oxide) are widely used to modify the optical properties of glasses. In particular, they allow to increase (or decrease) the absorption in the infrared spectral region. In our work, a method is proposed for determining the spectral absorption coefficient in the infrared range based on temperature measurements using thermocouples. The developed method of processing experimental data allows the use of a broadband (gray) radiation source. To estimate the spectral properties, a multigroup approximation is considered, according to which the spectral range is divided into intervals. Measurements are carried out in a vacuum chamber to avoid the influence of convective heat fluxes from the surface. To determine the integral absorption coefficient A, we considered the balance of absorbed radiation energy and the energy removed by the thermal conductivity through the sample under study. A comparison of the calculation with the results of the experiment shows their satisfactory agreement. Established measurement technique and experimental setup allow us to study various materials of substrates and coatings in the range of 5–20 μm, resulting in data on absorption coefficients and other spectral properties. The support of this study by grant from the Russian Foundation for Basic Research No. 17-08-01233 is gratefully acknowledged.

Optimization of the radio-transparent constructions in a mode of extreme heat loads

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Materials with basis SiO_2: fiberglass (STR-KM); reinforced quartz materials of SiO_2–SiO_2 (VRK-KM); silicone rubber with a mica filler (TPT) were studied according to the method [1] to optimize the composition of the layers of the radio-transparent constructions, working in extreme thermal loads. The parameters of thermal loads causing physical and chemical transformations in radio-transparent materials and significantly affecting the coefficients of transmission and reflection of electromagnetic waves, as well as the value of dielectric permittivity, are determined.
It was found that the reduction in the transfer coefficient after thermal irradiation for the VRK-KM is up to 3–4 dB in the frequency range from 2 to 40 GHz, and for TPT and STR-KM to 25 dB. Moreover, the strongest changes in the transmission coefficient are observed in the short-wave region of the spectrum. Thus, it is shown that the best indicators of radio transparency has a fairing, consisting of an ceramic composite material VRK-KM.

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Thermal action of pulse radiation on the carbon conic shells loaded with internal pressure

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The new mechanism for destruction of aircraft constructions from composite materials at thermal action of fluxes of radiations and particles (FRP) was offered in work [1]. It was assumed that operability of a construction is broken because of development of non-stationary processes of deformation and destruction under the action of quasi-stationary flight loadings. These non-stationary processes are formed by means of almost instant change of rigidity of a construction at pulse FRP-heating of materials.

Carbon nozzles of the working rocket engines of upper steps [2] is in hard heatstrength conditions. FRP is prevailing for upper steps in comparison with other factors of powerful explosion (for example action of a shock wave).

The maximum levels of pulse FRP of a Plank spectrum that safely for a model nozzle of the running engine are received as a result of systematic calculations by means of numerical model [3].

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New gasdynamic device for modeling of mechanical action of radiation

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Main method for a research of consequences of mechanical action of radiation [1] is test of constructions loading by gasdynamic devices. Development of set of such devices is actual and has great practical interest. It is well-known [2] that the available sets of the modeling devices do not provide generation of the low-pulse loadings having small duration and high simultaneity of action to the construction surface. But such non-stationary loadings are required for strength tests of thin-walled constructions at mechanical action of radiations. The original gas-dynamic device for generation of low-pulse actions of microsecond duration with high simultaneity of loading of a surface of the studied constructions was offered and tested. This device is a contact charge with the controlled initiation. The contact charge is produced in the form of thin (no more than 3 mm) covers from fibrous material. The milled channels filled with the plastic explosive are located in this cover. Its distribution in channels gives some advantages in comparison with other ways of localization of explosive.

The performed experiments show high stability and adequacy of reproduction for mechanical action of radiation by means of the offered device.

The work was made under support by the Russian Foundation for Basic Research (projects No. 16-08-01065, 18-08-00094).

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

[2] Ostrik A V *et al* 2008 *Mechanical x-ray action on thin-walled composite constructions* (Moscow: FIZMATLIT)

Modern set of devices and the unified stand for tests of constructions to thermal and mechanical actions of radiations and particles

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Creation of the flight vehicle (FV) which have a resistance to action of radiations and particles fluxes (RPF) of various physical nature [1] is required now. Tests [2] of real constructions of FV loaded by gas-dynamic devices for modeling of RPF action are the main method for a research of consequences of RPF irradiation. Development of set of such devices is actual and has great practical interest. Numerical researches of interaction of RPF and modern high-porous sheetings and also the analysis of the available experimental data are used for the formulation of the requirement to a set of the modeling devices. As a result the list of such devices was defined. Preliminary estimates of possibilities (the generated parameters of loadings and their adequacy to thermal and mechanical actions of RPF) of new set were made. The new unified test stand allowing to investigate joint thermal and mechanical action of RPF on FV constructions with simultaneous modeling of flight conditions is offered. Modern sources of fast heating (by powerful ir radiation, pulsed laser and microwave action) are applied in this stand. This work was supported by the Russian Foundation for Basic Research (grants No. 16-08-01065, 18-08-00094).

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

[2] Ostrik A V *et al* 2008 *Mechanical x-ray action on thin-walled composite constructions* (Moscow: FIZMATLIT)

Some strong field effects at high energies

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Quantum-electrodynamic processes in the strong electromagnetic field have been studied both theoretically and experimentally about two decades ago for electrons (positrons) interacting with the electrostatic fields of atomic axes (planes) in oriented crystals at the beam energies up to 270 GeV [1]. In this case, the value of the critical Schwinger invariant field parameter exceeds that of unity.
Designing of powerful tera and petawatt laser systems have opened up new alternative methods to study the strong field effects in the laboratory [2]. These two approaches turn out to have many similarities including photon emission [3], pair production [4, 5], radiation damping effects [6] and cascade processes [7].
We present strong field effects on radiation cross sections in laser fields and electrostatic fields of oriented crystals and demonstrate their discrepancies and similarities. The special realistic superposition of two laser beams has been considered, in which the magnetic field is suppresses and, on the contrary, the electric field is enhanced. The pair production is such combined strong laser field is studied.

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Determination of the feature of the Fermi surface of metals using low-background spectroscopy of the Doppler broadening of the annihilation line

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The results of experiments on the precise measurement of gamma spectra during the annihilation of thermolized positrons on metal targets are presented. The experiments were carried out in low-background conditions of the Baksan neutrino observatory using a semiconductor detector based on a single-crystal of extremely pure germanium 7×7 cm^2 in size [1]. The detector was placed in passive protection against thermal neutrons, beta and gamma radiation. A source of ^{22}Na with an activity of 2×10^5 Bq was used as a source of positrons. The Doppler broadening of the annihilation line is due to the fact that positron annihilation occurs on electrons moving with velocities of the order of Za for valence electrons and $v = P_f/m^* = \hbar(3\pi^2 n_e)^{1/3}/m^*$, where Z is the charge nuclei, $a = 1/37$, c is the speed of light, n_e is the concentration of conduction electrons. When annihilating positrons on the conduction electrons of Al, Ag, Pb, the Doppler shift amounts to 3–5 keV.

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Alpha-particles from p–^{11}B reaction at inertial electrostatic confinement

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In this paper, we present the first experimental results on aneutronic proton–boron nuclear synthesis ($p+^{11}B \rightarrow \alpha+^{8}Be^{*} \rightarrow 3\alpha$ [1]) in the field of a virtual cathode in nanosecond vacuum discharge (NVD) [2]. The formation of a deep quasi-stationary potential well provides in the interelectrode space both confinement and acceleration of protons and deuterons to energies of tens of keV, and multicharged boron ions—up to hundreds of keV [3]. This turns NVD into a kind of microreactor of "collisional" nuclear synthesis, including an aneutronic one [2]. In this experiment, as before, in the cylindrical geometry of the NVD [3], a new hollow cathode with slots along the axis was used, which made it possible to register the yield of α-particles both along the discharge axis and radially. Boron was applied onto Pd anode tubes with a developed surface microrelief using cataphoresis in aqueous suspension of boron nanopowder, and at the same time Pd tubes were saturated with hydrogen by electrolysis. The CR-39 detectors have registered reliably the excess of the α-particle yield over the background (five times) both along the axis and along the discharge radius. The features of tracks of α-particles on CR-39 are presented and discussed, depending on their location and screening with aluminum foil, which allows just for α-particles with energies $E \geqslant 3$ MeV to pass through.

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On the influence of the microwave treatment in the synthesis of selenium nanostructures

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Selenium, the second element of chalcogenide family (S, Se, Te) has some crystalline and amorphous modifications and a lot of wonderful properties, not yet discovered completely for a while. So red amorphous selenium has antioxidant properties and on this reason can be used as reagent with antibacterial, anticancer, antidiabetic action. But it is known nowadays these properties can be enforced sufficiently owing to nanostructural state of element, bearing in mind reduced toxicity of this modification also. The choice of surfactants used for preparation of nanoparticles is the very significant step of a research because they define the stability of the system, the time period of its existence. We had studied the formation and stability of selenium polymeric nanocomposites. Solutions of selenous acid, surfactants, sulfur dioxide were mixed in polymeric media. Microwave irradiation was used for activation of redox reactions in our systems. Solutions and polymeric films, obtained after drying of solutions were studied with optical, ES microscopy, UV-Viz, and Raman spectroscopy. Conclusions were made on the influence of microwave irradiation on the final nanocomposite produced in the course of the process studied.

Specifics of condensation processes of metal clusters in superfluid helium

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In the present work the processes of condensation of the products of laser ablation of metals in superfluid helium (He II) and in vacuum are investigated using tungsten as an example. According to the accepted model [1], the processes under consideration in both media are adiabatic, and yet the condensation products are strikingly different: spherical nanoclusters in the case of vacuum giving way to the long quasi-one-dimensional structures (nanowires) in the case of He II. To reveal the differences in the mechanisms of condensation processes, special experiments on observing the thermal radiation accompanying the condensation of tungsten clusters were carried out. It turned out that although condensation in both cases occurs at high temperatures comparable to the melting point of tungsten, in the case of He II it possesses much faster kinetics, which can be explained by the concentration of metal nanoparticles in quantized vortices, which thereby play a special role in condensation processes.
The work is financially supported by the Russian Science Foundation (grant No. 18-19-00620).

[1] Gordon E B, Kulish M I, Karabulin A V and Matyushenko V I 2017 *Low Temperature Physics* **43** 1086–1093

Spin waves induced by ultrafast spin-polarized carrier transport in Fe–Au–Fe structure

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Approaching the timescales of the underlying elementary processes, spin currents (SCs) with femtosecond pulse duration [1] can provide valuable fundamental insights into the ultrafast spin dynamics. In addition to manipulating the magnetization in multilayer structures [1], ultrashort SC pulses were shown to exert spin transfer torque (STT) and thus drive the coherent magnetization dynamics in semiconductor films, or perpendicularly coupled magnetic bilayers. Complementing static or frequency domain studies, this time domain approach employs quasi-instantaneous driving of collective magnetic excitations by ultrashort SC pulses thus providing access to coherent spin dynamics. Aiming at understanding characteristic microscopic STT length and timescales, we address this challenge by studying spin dynamics in considerably thicker FM layers. The analysis of their importance and the relevant length scales is the major aim of our work. We realize this approach in epitaxial Fe–Au–Fe–MgO(001) multilayers by means of optical detection of the standing spin waves in a 15-nm Fe film excited via the STT mechanism. We demonstrate the complex mode structure of the excited non-uniform magnetization dynamics and show that the ultrashort laser-induced SC pulses constitute a convenient tool to excite spin waves and study the interaction of spins with a non-collinear magnetization.

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The resonant properties of dielectric magnetic dipoles in the form of a ring and an ellipse at different angles of incidence of electromagnetic wave

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The aim of this paper was to investigate the amplitude and possible shift of the resonance frequency dependence on the angle between the plane of dielectric magnetic dipoles in the form of a ring or an ellipse and the magnetic field vector and to check the theoretically predicted disappearance of scattering at zero angle between the plane of the ring and the magnetic field vector. The network analyzer Agilent E5071C ENA was used to generate and record the emission spectra of the GHz band. The magnetic field was recorded by a shielded probe with a sensing circle element diameter of 3.8 mm. Magnetic response measurements for the ring with dimensions of $38 \times 28 \times 5$ mm and ellipse with dimensions of large and small axes of 51 and 11 mm, respectively, and rectangle cross-section of 5×7 mm were made every 10 degree. The experimental data showed that the resonance frequency of magnetic dipole does not depend on the angle of rotation of the dielectric ring relative to the magnetic field vector. At the zero angle of the dipoles plane location to the magnetic field vector, the signal of the main resonance frequency disappears, which corresponds to the results of numerical simulation. The work was supported by the Russian Foundation for Basic Research, grant No. 18-08-00633.

Linear dielectric ring structures in a plane electromagnetic wave field

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The resonant structures with different number of elements consisting of dielectric magnetic dipoles in the form of linearly arranged dielectric rings excited by a plane electromagnetic wave in the microwave frequency range at a sliding incidence of a plane wave are investigated. The network analyzer Agilent E5071C ENA was used to generate and record the emission spectra of the GHz band. The dielectric rings used in these experiments with a diameter of 16 mm and a cross-sectional area of 3×3 mm are characterized by a dielectric constant of 170. Spectral measurements showed that the frequency of the main resonance of one ring is 2.43 GHz, its half-width is 20 MHz. Numerical simulation and experimentally showed an increase in the half-width of the peak of the resonance frequency from 20 to 200 MHz with an increase in the number of rings to 4 pieces. It should be noted that an increase in the number of rings in the linear chain leads to an increase in the depth of the resonance absorption of the incident radiation. It is found that the results of numerical simulation are in good agreement with the experimental results. The work was supported by the fundamental research program of Presidium of RAS No. 13 “Condensed matter and plasma at high energy densities”.

Scattering of plane electromagnetic waves in GHz range of frequencies by a dielectric ball and dielectric cylinder

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Scattering of plane electromagnetic waves by subwavelength dielectric elements in the form of a ball and a cylinder with a high dielectric permeability of the order of 170 are investigated. These elements make it possible to obtain a negative magnetic response at a resonance frequency in the microwave range, which can be recorded using a magnetic field probe, the size of which is smaller than the element under investigation. In the region of the main magnetic resonance, these elements look like magnetic dipoles. In the case of a ball this is the so-called first resonance of Mie, in the case of a cylinder this is the resonance on the main magnetic mode. With magnetic resonance, the circular bias currents in the dielectric amplify the magnetic field at the center of the particle. In the cylinder, the resonance on the main magnetic mode is stronger and has a narrower dispersion curve than that of the ball. The resonant frequencies of a dielectric ball and a cylinder of the same volume were measured. Their main resonant frequencies differ by more than 1.5 times, which coincides with numerical calculations. The use of dielectric resonators with negative magnetic permeability makes it possible to create ideal reflectors and magnetic mirrors with very small losses, both in microwave, and in the ir and visible frequency range.

Behavior of heavy metal during pyrolysis in the composition of sewage sludge

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One of the sewage sludge characteristics is the presence of various pollutant types. This is both pathogenic microflora and chemical pollutants, for example, heavy metals. When using the pyrolysis process up to 800 °C with thermal cracking of volatile products, as a method of processing sewage sludge described in [1], in addition to synthesis gas a solid residue is formed. According to previous studies, the solid residue is about 40% by weight of the initial sewage sludge and has an ash content of 58.2% on dry state [2]. With this amount of ash, the use of solid residue for energy purposes is not appropriate. Such material is subject to disposal. In this connection, the question arises, what proportion of heavy metals remains in the solid residue and goes into synthesis gas. In Russia, the Ministry of Natural Resources and Ecology controls the total content of nine heavy metals in the soil. They are V, Mn, Pb, Cd, Cu, Ni, Zn, Co, Cr. This paper presents the study results of the effects of pyrolytic processing conditions on the behavior of these heavy metals in the composition of sewage sludge. The total content and solubility in neutral and acidic media of heavy metals in the composition of the initial sewage sludge and the solid residue from pyrolysis are determined. The hazard class of the initial sewage sludge and the solid residue according to the content of heavy metals is calculated.

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[2] Larina O and Zaichenko V 2018 *J. Phys.: Conf. Ser.* **94** 1–10

Two-stage pyrolytic conversion of raw and pretreated bagasse into synthesis gas

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Sugarcane bagasse is one of the largest cellulosic agro-industrial by-products. It is a fibrous residue obtained after the extraction of the sucrose-rich juice from the sugarcane stalks. Sugarcane annual global production of approximately 1.6 billion tons generates several hundred million tons of bagasse. It is estimated that for every 3 kg of cane crushed, 1 kg of bagasse is produced. Finding the best ways for processing bagasse is currently an urgent task. The article presents the data obtained using the method of two-stage pyrolytic conversion developed at the Joint Institute for High Temperatures. Raw bagasse has high moisture content and hygroscopic nature, so it is prone to chemical biodegradation. Raw bagasse as well as pretreated bagasse obtained by torrefaction and hydrothermal carbonization, were used as initial materials for the conversion to synthesis gas. Experimental data are presented including composition and quantity of gaseous products. Combustible components content is 97, 98 and 96% for raw, torrefied and hydro carbonized bagasse, respectively. The gas yield in the processing of torrefied and hydro carbonized bagasse is 12 and 15% lower compared to the raw bagasse, respectively, and ranges from 0.93 to 1.26 m^3/kg. Lower calorific value ranges from 10.78 to 10.96 MJ/m^3. This work was supported by the Russian Foundation for Basic Research (grant No. 17-08-01393).

Development of an experimental unit for two-stage thermal conversion of pulp and paper industry waste into high-quality gas

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The results of the thermotechnical calculation of the experimental unit "Pyroenergy-300" with a capacity of 300 kg/h for raw materials (moisture content 48%) intended for the thermochemical processing of pulp and paper industry waste into high-quality gas are presented. The unit operates on the principle of two-stage pyrolytic conversion, combining the pyrolysis of raw materials and the subsequent high-temperature cracking of volatile products in a fixed bed of coke residue. Calculation based on previous studies [1, 2]. The result of the calculation of the main processing indicators:

- specific gas yield—0.73 m^3/kg;
- total volume fraction of combustible components—98%;
- lower heating value—11.2 MJ/m^3;
- thermal power output—685 kW;
- the efficiency of conversion of raw materials into gas—68.2%;
- the amount of ash and unburned coke residue—5.4 kg/h.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation (project No. 14.607.21.0197, unique identifier RFMEFI60717X0197).

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Research of technologies of local fuel and energy resources using for distributed power generation

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Development of methods of energy self-sufficiency is a priority for present power generation sector advancing. For our country, it is of particular importance. Approximately 70% of the territory of Russian Federation (with a population of about 20 million people) are outside centralized energy supply systems. Capacity of existing centralized energy systems is not enough for many regions of the country. At the same time, in the existing economic conditions, distributed power generation turns out to be more advantageous from an economic point of view in relation to centralized power generation. The production of energy without imported organic fuels implies local fuel and energy resources using, such as peat, wood, agricultural, household and other types of waste. Energy utilization of various types of waste, which are also local fuel and energy resources, will reduce the negative impact on the natural balance of accumulated environmental damage.

In this paper results of research of methods of organic waste energy utilization with subsequent production of various fuel and energy resources: synthesis gas, conditioned solid hydrocarbon fuel, and carbon composite. It is concluded that further tests are needed to assess the feasibility of the industrial implementation of proposed approaches.

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Effect of temperature on the torrefaction of biomass in the quiescent layer of mineral filler

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The use of biomass as a fossil fuel is an important task, due to the need to solve a number of environmental problems. However, its low energy density do not allow biomass to compete with traditional petroleum based or coal fuels. Torrefaction technique is used to improve the properties of biomass. Torrefaction is the process of low-temperature pyrolysis of biomass with limited oxygen content or without oxygen at all. Current study is devoted to the effect of temperature on the properties of biomass obtained using the new technique of torrefaction in the quiescent layer of mineral filler [1,2]. Based on the experimental data, it can be concluded that at low temperatures (220–230 °C), there is a noticeable deceleration in the process of depolymerization of the main components of biomass, although the oxidation reactions remain to be active. The intensity of torrefaction at low temperatures is determined only by the kinetics of chemical reactions and does not depend on the diffusion resistance of mineral layer. The duration of torrefaction process and the type of wood biomass become important. At high temperatures (280–300 °C), the rates of chemical reactions do not play a significant role since the rate of the process is determined mainly by the diffusion of oxygen through the mineral layer. It is shown that the mass yield can vary with the characteristics of the mineral layer such as height of the layer and porosity of the mineral layer.

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Effect of temperature process at chicken litter torrefaction on properties of products obtained

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Due to the environmental and energy situation in the world, it is necessary to study the possibility of bio-waste using as energy resource. The method of thermochemical treatment of organic waste is investigated in this paper. The chicken litter in the form of pellets is used as a raw material. The experimental studies of the torrefaction temperature influence on the thermotechnical characteristics of chicken litter and the yield of products were conducted in lab-scale system. The five temperature regimes of torrefaction (220, 240, 260, 280, and 300 °C) with holding time determined with thermogravimetric analysis are studied. The thermotechnical characteristics of the initial and torrefied material as elemental composition, the lower calorific value, hygroscopicity limit, and bulk density are determined. The properties of non-condensable gases (specific volume yield, chemical composition, and calorific value) are investigated. The material balance for each of the temperature regimes is calculated. The conclusion about the optimum temperature regime for torrefaction of chicken litter based on the results of experimental studies are made.
The study was carried out by a grant from the Russian Science Foundation (project No. 18-79-00286).

The properties of biocoil made of chicken litter by methods of torrefaction and hydrothermal carbonization

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Recently, the problem of animal waste utilization has become quite acute in the world. Volumes of meat consumption are growing, but there is no general-purpose technology, that could be able to recycle animal waste with a value-added product producing.

In this paper the possibility of chicken litter processing by hydrotermal carbonization (HTC) and torrefaction was studied. HTC and torrefaction are modern low-temperature methods of improving characteristics of biomass of different origin a product disposal methods. Hydrothermal carbonization (HTC) is carried out in anaerobic conditions in the presence of subcritical, liquid water. It proceeds usually at temperatures ranging from 180 to 280 °C [1].Torrefaction or dry mild pyrolysis is a low-temperature peat processing that is carried out in anaerobic conditions in the absence of water. The biomass moisture schould be reduced down to 15%. Temperature of torrefaction is slightly higher then HTC one. Process proceeds at 200-300 °C and atmospheric pressure [2]. The influence of methods at different temperatures on the physicochemical and energy properties of the resulting biocoil is studied.

The research was financial supported by the Russian Foundation for Basic Research (grant No. 17-08-01393).

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Nonsingular stable black holes, holding the baryon conservation law in the periodic waveguided multiverse

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Nonsingular stable black holes (BHs), arising in the periodic waveguided multiverse (PWM) concept by the author, are compared with singular BHs in Einsteinian general relativity (GR). The PWM is a four-dimensional periodic chain of identical quasi-flat three-dimensional (3D) waveguides physically identical 3D-universes. The united wave-dynamical special relativity, weak Newtonian gravity and equivalence principle, quantum mechanics and nonsingular quantized massive fermions, including nonsingular matter-BHs, antimatter white-holes (WHs), dark matter (DM) and dark antimatter (DAM) BHs are co-emergent in the nearest 3D-waveguides 3D-universes of the PWM. Notably, the PWM-BHs have identical Schwarzschild-like radiuses as in the GR-BHs (but they are nonsingular), have identical, totally flat gravity potentials, zero gravitational field strength inside. The PWM-BHs nonsingularity corresponds to the PWM-emergent hollow-nonsingular elementary quantized massive fermions. They cannot create microscopic BHs (formally possible in the GR for point-like particles), only very heavy PWM-BHs can arise inside stars. This automatically rejects the famous Hawking's strongly radiating mikro-BHs concept, never verified experimentally on colliders. The plasma-eating (growing PWM-BHs are positrons factories) radiate positrons and antiphotons, plenty of positrons where observed in the middle of galaxies; but the isolated PWM-BHs are electrostatically self-stabilized in the vastly dominating weightless superfluid PWM-vacuum-medium.

2. Shock Waves, Detonation and Combustion

Polymetodical measurements of high-speed processes

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In connection with the progress in the field of mathematical modeling of high-speed processes, one observes strengthening of requirements to informative value and accuracy of gas-dynamic experiments. Achieving high accuracy of experimental results only at the coast of increasing the number of experiments might be economically unpractical, and in some cases, it would be impossible. Improving reliability of experimental results is achieved by increasing information scope, which is obtained in experiments and by using up-to-date precise methods of measurements. However for some tasks, of importance is preserving consistency of measurements that permits to conduct direct comparison with experimental data that were obtained earlier. In this case, the scope of experimental information that was obtained by standard method is supplemented by experimental results from one of several additional techniques. Using methods that function on various physical principles permits to mitigate weak sides of one technique by advantages of other techniques and to increase information value at the coast of measurement of several gas-dynamic parameters for investigated phenomenon in one experiment.

This work demonstrates the examples of several techniques for investigation of high-speed processes, consider providing their united functioning synchronizing. For solving arising problems, proposed polymethodical approach to measurements permits to rationally select both existing and promising techniques in combination regime.

Synchronous diagnostics for the processes of twofold shock compression

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Unique features of synchronous radiation open wide possibilities of its application for vizualization high-speed processes. High periodicity of synchronous radiation, low duration of pulse and low angle divergence of probing radiation permit to conduct precise noninvasive diagnostics of shock-wave phenomena, including the processes of multiple interactions of shock waves and rarefaction waves.
The work presents the set-ups and the results of experiments, which realized the regimes of shock waves reflection from a barrier and collision of oncoming shock waves. Registration of the processes of incident shock waves motion, collision and formation of reflected shock waves was performed using synchronous radiation. Experiments were conducted on acceleration complex VEPP-3 at the Budker Institute of Nuclear Physics SB RAS.

The project station "Fast Processes" based on the Siberian Ring Source of Photons

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Within the framework of the Center for Collective Use (CCP) of the Siberian Ring Source of Photons (SKIF), a station "Fast Processes" is created The experimental station is designed to study high-speed processes in functional materials, as well as the behavior of matter and materials under conditions of powerful pulsed effects of laser radiation, explosion, shock waves, plasma and directional particle fluxes, and in the synthesis of new high-temperature composite materials and catalysts.

The project of the station is aimed at developing methods for using synchrotron radiation (SR) for the study of fast processes (including using energy materials—EM) and obtaining direct experimental data in new materials (EM, catalysts) with various shock-wave effects on them (including powerful EM). The measuring equipment will be optimized for x-ray, spectral and diffraction measurements with high temporal resolution, up to the registration of a signal from each bunch (less than 5 ns).

A distinctive feature of this project is the complexity of the use of different methods for measuring compression parameters.

The structure of the station "Fast Processes" includes the following experimental sections: 1—"Dynamic Processes"; 2—"Plasma"; 3—"Extremely High Temperatures".

Dynamics of supernova bounce in laboratory

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We draw attention to recent high explosive (HE) experiments, which provide compression of macroscopic amount of matter to high, even record, values of pressure in comparison with other HE experiments. The observed bounce after the compression corresponds to processes in core-collapse supernova explosions after neutrino trapping. Conditions provided in the experiments resemble those in core-collapse supernovae, permitting to use them for laboratory astrophysics. A unique feature of the experiments is compression at low entropy. The values of specific entropy are close to those obtained in numerical simulations during the process of collapse in supernova explosions, and much lower than those obtained at laser ignition facilities, another type of high-compression experiments. Both in supernovae and HE experiments the bounce undergoes at low entropy, so the HE experiments provide a new platform to realize some supernova collapse effects in laboratory, especially to study hydrodynamics of collapsing ows and the bounce. Due to the good resolution of diagnostics in the compression of macroscopic amounts of material with essential effects of non-ideal plasma in equation of state, and observed development of tree-dimensional instabilities, these experiments may serve as a useful benchmark for astrophysical hydrodynamic codes.

Central engines of superluminous supernovae and their environment

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Recently, a new class of superluminous supernovae (SLSNe) is discovered. They have luminosities a factor of 10 higher than ordinary supernovae (SNe). Large amounts of mass may be expelled by a star a few years before a supernova explosion. The collisions of SN-ejecta and the dense circumstellar matter may provide the required power of light to make the supernova much more luminous. This class of models is referred to as "interacting SNe". The propagation of radiative shocks and formation of dense shells involve many instabilities which are analyzed in our two- and three-dimensional hydrodynamic simulations taking into account important physical effects.

Many SLSNe-I have photospheric velocity of order 10^4 km/s, which is hard to explain in interacting scenario with modest energy of explosion. A strong "hypernova" explosion improves the situation and the properties of SLSNe near maximum light are explained by a gamma-ray-burst-like central engine, embedded in a dense envelope and shells ejected prior the final collapse–explosion of a massive star. In this case velocity up to 1.5×10^4 km/s is no problem. The problem remains with the nature of the central engine and evolution scenarios leading to double explosions.

Problems of impact craters formation in the light of recent lunar missions

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The report discusses various aspects of the impact formation of large lunar craters, seas and mascons, which allow better understanding of this process physics. To this end, we are analyzing the results of the latest missions of the Moon exploration by new high-precision methods. These are orbital pictures of the lunar surface of high and super high resolution (the Lunar Reconnaissance Orbiter); laser altimetry and inter-satellite tracking methods (the Gravitational Recovery and Interior Laboratory), as well as expected results of the Chinese lunar station (the Chang'e-4). Based on high-resolution images, we have built 3D-models of large impact craters, which allow revealing new effects that accompany shock events of different power and age. As result of comparing large craters on Moon with similar impact structures on Mars and Mercury, it was concluded that lunar craters can play a significant role in the theoretical study of the impact processes physics in Solar System as a whole. Therefore, from the point of view of the impact processes physics, Moon should be regarded as an excellent "natural laboratory", which has a rich set of impact craters for its research.

A fluid dynamical model for the shape of complex craters

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A simple and effective tool has been developed for the description of the physical process of crater formation, as well as its resulting shape after the body fell to the surface of an atmosphereless planet. The basis of the development is a fluid dynamic theoretical model. Several stages are highlighted and considered in the process of cratering in order to apply the newly developed shock wave front pattern [1]. Time, geometry and speed are determined using the laws of conservation of mass, momentum balance, conservation of total energy and the first law of thermodynamics in each of them. The three-dimensional model of the 3D-HM hose, the GCGM global crater formation model and the central lift model, CUGM have been proposed for the understanding and the explanation of crater formation. The state of the art is improved after the application of the new shock wave pattern, by its postulation of physical stages, each with its initial and boundary conditions, and the adaptation of complementary models to fluid dynamical laws. To conclude, all of these new analytical tools seem to be promising for the prediction of craters formation and description of their shape. We think that in the future, further predictions from the given models should compare with high-resolution images of craters for any celestial body [2].

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Shock treatment of porous cubic zinc sulfide

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Despite the fact that compaction of porous hard and brittle materials is of great interest to the research field, its dynamic behavior at high loading rates has not been fully studied [1]. To get better insights in these problems first experiments with volatile rich synthetic synthetic cubic zinc sulfide were performed. It is comparable with many hard materials, because it shows a (not recoverable) phase transition into a rock salt-type phase [2], it is able to show chemical decay reactions and its Hugoniot–equation of state in the solid phase is already well described [3] if an impedance correction of the recovery capsule is required. In a first set of experiments we have recovered almost wurtzitic ZnS in dependence on the initial porosity of the sample under comparable pressures (charge masses). In this case the results are comparable with synthesis by Petrov *et al* [4]. The internal structure of the sample and its melting behavior depends strongly on the materials of the recovery capsule and by the occurence or absence of internal reflections and partial adiabatic decompression.

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On interaction of metastable shock waves with perturbations

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The shock waves, which correspond to the segment of an ambiguous representation of the shock-wave discontinuity that overlaps the instability $L > 1 + 2\mathrm{M}$ segment on the Hugoniot, are shown to exhibit metastable behavior. Namely, beyond the instability region these shock waves interact with small perturbations like stable ones. However, if the perturbation amplitude exceeds a certain critical value, multidimensional shock wave instability develops. The critical amplitudes of the perturbations vanish when the postshock state approaches the instability boundary. The problem of interaction of the metastable shock wave with compact entropy perturbation passing through the shock-wave front is studied in the framework of 3D problem formulation. The instability development and transition of the shock wave to the limiting self-oscillating mode are described. The instability development and transition of the shock wave to the limiting self-oscillating mode are described. The instability is accompanied by the formation of "switching" secondary waves. The local post-shock states in this waves partly belong to the lower and partly to the upper stable branches of the Hugoniot separated by the instability segment. The secondary waves of this kind propagate along the primary shock wave at constant amplitude. Taking into account the characteristic features of the phenomenon, the metastable behavior of the shock wave may be served as marker of fulllment of $L > 1 + 2\mathrm{M}$ shock wave instability condition. The work is supported by program No. 13 of the Presidium of the Russian Academy of Science "Condensed matter and plasma at high energy densities".

Study of plasma and particles flow escaping from metal target

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This article is a continuation of the previous works of the authors [1, 2]. The authors developed a special technique and used it to measure surface temperature in flat [3] and cylindrical installations, the latter using three different methods. In this study, the authors observed the particles ejection and plasma formation process that unfolds on the line between copper target and partial vacuum containing residual gas (air) when a strong shock wave reaches free surface of the sample. Experimental facilities included linear explosive generator and setup with an option to lateral observation (transit time registration technique). Thermal radiation was measured by three channel high-speed pyrometer (wavelength 650, 820 and 960 nm; bandwidth 40, 10 and 10 nm respectively). Radiation intensity was adjusted to tungsten filament lamp calibration and optical losses. Plunger velocity of around 5 km/s caused particles and plasma flow escaping from the target surface at maximum flow front velocity of around 12.5 km/s.

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Dusting of samples impacted by the laser pulses using the photon Doppler velocimetry technique

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Currently, one of the most common and actively developing methods for measuring particle velocity is the photon Doppler velocimetry (PDV). This technique allows continuous measurement of the target velocity.

A series of experiments were conducted on the Kamerton-T facility in coherent radiation interaction department of the Prokhorov General Physics Institute of the Russian Academy of Sciences. Shock-wave loading was carried out by laser pulses. The laser pulse energy: 1 J, the radiation was focused on the target into a spot with a diameter of 0.4 to 3.7 mm, the maximum laser radiation flux density in the focusing region reached 1.6×10^{13} W/cm^2. Aluminum and lead plates with a thickness of from 50 to 200 μm were used as targets. Targets were in a vacuum chamber.

As a result, velocity profiles were obtained for various parameters of the laser pulse. The time of the wave to reach the sample surface coincided with the theoretical calculations of the error limits, which indicates the applicability of this technique.

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Sound velocity measurements of shock-compressed epoxide resin by the photoelectric registration technique

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The paper presents results of the sound velocity measurements by the overtaking release method used with shock-compressed samples of the EK-34 epoxide compound in the pressure range from 16 to 38 GPa. The loading explosive devices based on powerful condensed explosives with steel impactors at flight velocities ranging from 2.7 to 4.8 km/s were used to produce the shock waves in the samples. The signals were recorded by photoelectric registration technique. The obtained results of measured sound velocities in shock-compressed epoxide resin are compared to the previously published data.

Vernier line-imaging VISAR for shock processes investigation in matter under the influence of intense laser pulses

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The paper presents the diagnostic system for velocity measurements of reflecting objects in laser-driven shock-wave experiments. The principle of continuous velocity measurements based on the Doppler frequency shift analysis of a probe monochromatic wave reflected by the moving surface of the sample. This diagnostic method is non-contact and provides information about the object with high spatial and temporal resolution.

The system is designed to measure speed in the interval from 5 to 50 km/s and consists of 3 separate parts: optical stand with interferometers, probe laser for target illumination and control computer. Optical system based on two tine-imaging Mach-Zehnder interferometers, that form a vernier measuring system. Registration is performed by streak cameras with time resolution about 10 ps.

Probe light source is a pulsed Nd:YAG laser at a wavelength of 660 nm (2nd harmonic of 1320 nm). Probe laser consists of CW seed laser diode, Nd:YAG master oscillator with stabilized cavity and amplifier. This scheme allows obtaining the single-mode pulse with energy of 30 mJ, time duration 100 ns with the frequency up to 10 Hz. Laser and optical stand connected by 40 meters of 1-mm optical fiber.

Multipoint shock wave experiments combining the VISAR and the photon Doppler velocimetry techniques

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Currently, the most common way to study the strength properties of a substance is the shock-wave technique for high-velocity impact. In the study of shock-wave processes, each experiment is unique in its own way and has a number of hardly reproducible parameters. The main parameter available for measurement in these experiments is the mass velocity. The most popular methods for recording the high speed in experiments of this kind are the VISAR and the photon Doppler velocimetry (PDV). The paper presents the results of a joint experiment, where the speed of aluminum samples was measured simultaneously by two instruments: KIWI (PDV) and KDNI 532-7 (VISAR). To solve the problem of continuous research of the fragmentation processes and dusting of objects with the use of the PDV technique. The obtained profiles demonstrate the coincidence of nature of the dependencies of two different measurement methods within the limits of error. The presented systems allow to make multichannel measurements of the mass velocity of a high value. The combination of two methods when sharing the two systems allows to increase the reliability and accuracy of the data on the temporal dynamics of the mass velocity. This work was supported by the Russian Science Foundation (grant No. 17-72-20164).

Vernier laser diagnostic system for velocity measurements at the Angara-5-1 facility

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Shock wave experiments are currently the main source of empirical data, that used for constructing equations of state of matter at high pressures. The Angara-5-1 installation generates voltages up to 1.5 MV and currents up to 6 MA, allowing accelerate the flyer by a magnetic field to speeds over 10 km/s. The flyer can be used as a plate for conducting shock-wave processes. The report presents a laser diagnostic system designed to measure the mass velocity and propagation of shock waves in a substance. For measurements, two interferometers were used: a push-pull VISAR and a conventional VISAR. The vernier recording system is organized by using the simultaneous measurement of speed with two interferometers with different delay lines (the delay line of the push-pull VISAR is 1280 m/s per band, for the conventional VISAR is 7730 m/s per band) to eliminate the ambiguity of determining the speed when it drastically changes. As a result of the experiments, the velocity profiles of the samples under study were obtained depending on the applied voltage. The obtained profiles correspond to theoretical calculations within the limits of permissible errors.

Explosive technologies for tests of constructions on strength to side pulse loadings

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Explosive devices for generation of pressure pulses are widely used for tests on strength of aircraft constructions. Current trend of development of these devices is creation of low-pulse generators of microsecond duration with high simultaneity of the applying of loading to a surface of the tested constructions. The tape charge and charge having the operated initiation are represented by the most perspective among such devices.

The tape charge is made of tapes of the explosive which are placed on tubes of round section. Tubes are equidistanted from a surface of the loaded object. The multipoint system for initiation of end faces of explosive tapes is used for improvement of simultaneity of loading.

The charge having the operated initiation is produced in the form of thin (less than 3 mm) shells from fibrous material with the milled channels filled with the plastic explosive. Placement in channels gives some advantages in comparison with other ways of localization of explosive.

Results of validation of modern devices for generation of pressure impulses are given. The considered set of devices is used for strength tests of thin-walled constructions when action of the directed fluxes of energy of various physical nature takes place.

The work is made under support of the Russian Foundation for Basic Research (project 18-08-00094).

Experimental study of spall strength of silicon rubber with microspheres under shock-wave action

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In the paper, porous media are studied using Si rubber with glass microspheres as an example. There were investigated three types of silicon rubber samples featuring different concentrations and sizes of microspheres: non-porous silicon rubber, porous silicon rubber with calibrated glass microspheres and porous silicon rubber with glass microspheres having a wide range of sizes. The density of the samples was 0.99, 0.55 and 0.48 g/cc, accordingly. The velocity profiles were measured with a VISAR laser Doppler interferometer. Investigating spall strength under pulse tension shows that the destruction beginning threshold of the samples in question is quite low. For the non-porous sample, it is around 30 MPa, for the porous ones it is an order of magnitude lower. The spall plate does not come off the sample after the beginning of destruction. The ability of the free surface velocity to change in such a way is typical for materials with a low destruction threshold. Moreover, the destruction is viscous and it does not cause "main crack" formation, the damage areas are isolated from one another and the spall plate remains connected with the sample, this connection slowing the separation down. Such destruction mechanism is typical for elastomers and heterogeneous materials with a polymeric binder; this mechanism is described within the framework of the viscous model of destruction.

The experimental study of deformation character of spheroplastics under shock compression

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The results of an experimental study of shock compression of samples modeling media with a given porosity are presented. Samples of spheroplastics were made of epoxy resin filled with glass microspheres, the volume concentrations of which were 0.20 and 0.45 volume fractions. Using the VISAR method, the motion profiles of the free surface of the samples in the pressure range almost completely covering the range in which there is a two-wave structure of the shock compression wave are measured.Shock adiabats in the pressure range of shock compression 0.13–1.17 GPa were obtained. The pressure of shock compression, at which the destruction of microspheres—0.08 GPa begins, is determined. The dependence of the deformation character on the concentration of microspheres in the sample was found.

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Investigation into detonation propagation in high explosive samples based on TATB and HMX

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This work presents experimental results of investigation of the velocity and shape of detonation wave front propagating in cylindrical high explosive (HE) samples that differ by the nature of explosive filler. We investigated explosive compositions based on TATB, HMX and mixture of the fillers out of TATB and HMX. Binding component in all explosives was fluoropolymer bond. Investigations of detonation rate and front shape of mentioned HEs were performed on cylindrical samples in the range of diameters 10–250 mm; this range was varied for each HE with regard for their critical detonation diameter. Initiation of HE samples under study was carried out by divergent detonation wave. Investigation of HE detonation velocity was performed using electrocontact technique. High speed photo recorder with linear gap scanning registered time profiles of detonation wave arrival to the edge sample surface; these profiles were translated into the shape of detonation front with regard for registered values of detonation velocity. Analysis of the results obtained in this work permitted to get the dependences of stationary detonation velocity (D_{st}) and the curvature of detonation front (k) on the diameter of the samples (d) for HEs under study. As the result of approximation of experimental dependences of D_{st} and k on the value of reverse diameter ($1/d$), we got the values of ultimate detonation velocity. We also diagnosed the influence of filler material portion on the values D_{st} and k.

Effect of the shell dynamic rigidity on the detonation propagation in plane charges of low-sensitivity TATB-based high explosive

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Characteristics that are responsible for the detonation properties of a high explosive (HE) include detonation critical thickness, detonation front shape, and size of the chemical reaction zone. These are variable parameters and they are controlled by different factors associated with both HE fabrication processing and conditions of this HE application. Presence of the shell plays a key role in the value of these characteristics. The effect of the shell and its dynamic rigidity on the detonation propagation in plane charges of a low-sensitive TATB-based HE including various initial porosity of the HE are investigated in this work. The required porosity of the HE items was obtained by pessing. The following materials were selected for the experimental study: plexiglass, fluoroplastic, aluminum, beryllium, magnesium, and copper. Dependence of the critical detonation thickness on the porosity of the studied low-sensitive HE was obtained in the experimental study. The effect of the shell dynamic rigidity on the value of the detonation critical thickness and the detonation front evolution are demonstrated.

Investigation into deformation of stainless steel fabricated with help of additive techniques, by method of Hopkinson composite rods in the range of strain rates 10^2–10^3 s^{-1}

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This work gives the results of investigation into dynamic properties of structural material—stainless steel fabricated according to additive technique, by three-dimensional (3D) printing method. Investigations were performed with the help of method of Hopkinson composite rods. This method permits to conduct tests for wide variety of materials, to study dynamic diagrams of compression and expansion in the range of strain rates 10^2–10^3 s^{-1}. Samples of stainless steel (12X18N10T analog) were fabricated by method of metallic powder laser sintering (Selective Laser Sintering) on industrial 3D-printer Realizer SLM-100-200. In the course of studies, 12 experiments were performed with the samples out of stainless steel. The range of impactor velocities was from 7 up to 14 m/s, while proper strain rates were from 0.75×10^3 up to 2.8×10^3 1/s. The work gives the diagrams stress–strain and velocity strain–strain.

Features of the processes of elastic deformation in cubic crystals

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The mechanical properties of anisotropic materials, which include single crystals with cubic symmetry of properties, depend on the direction.
When they are loaded in some directions, a common feature is auxeticity (deformation of the same sign in the direction perpendicular to the direction of loading).
In single crystals of cubic symmetry, the elastic properties in the (011) plane are traditionally investigated.
This is due to the presence of negative Poisson's ratios (auxeticity), and also values exceeding 0.5 and even 1.5 for some types of single crystals.
The elastic properties coincide only when the axes are rotated by an angle of 90° in the (011) plane. For any other angles of rotation in the (011) plane, the elastic properties are different.
Therefore, when the direction of shock loading is changed relative to the crystallographic axes of single crystals with cubic symmetry of properties, and also when the computed coordinate system rotates at least in one plane relative to the crystallographic axes, the wave pattern of deformation in such single crystals changes.
On the example of solving a test problem (Taylor test) with different orientations of crystallographic axes of a single crystal with cubic symmetry of properties relative to the cylinder axis in a three-dimensional formulation, features of the deformation processes characteristic of auxetic materials are shown.
Investigations were conducted with the dynamic finite element method using original programs.
The study was carried out at the expense by grant from the Russian Science Foundation (project No. 18-71-00062)

Elastoplastic deformation processes in materials with cubic symmetry of properties

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Elastoplastic deformation of materials characterized by cubic symmetry of properties depends on the direction of loading relative to the axes of symmetry of the material. The propagation of longitudinal and transverse waves for such materials is possible only along three directions: [001], [011] and [111]. The elastic and plastic properties in natural experiments are investigated along these directions. As a rule, materials characterized by cubic symmetry of properties have auxeticity (deformation of the same sign in the direction perpendicular to the direction of loading), strongly pronounced anisotropy of Young's modulus and yield strengths.
The paper is presented an analysis of the features of deformation of a single crystal alloy VZHM8, which has a cubic symmetry of properties, under dynamic loading. The directions of shock loading are considered as directions [001], [011] and [111]. The following directions [001], [011] and [111] are considered as shock loading directions. The anisotropy of the elastic and plastic properties of VZhM8 is taken into account, and also the dependence from the direction of the velocities of propagation of elastic and plastic waves. It is shown that with an initial shock loading speed of 50 m/s in a cylinder made of VZhM8 alloy, the maximum elastoplastic deformations differ by 4 times for different loading directions. The calculations are carried out with the finite element method.

Influence of auxeticity on the processes of elastic deformation in a single crystal VZhM8 in the direction [011]

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Single crystal heat-resistant nickel alloy VZhM8, used for the formation of the blades of a gas turbine engine V generation, has a cubic symmetry of properties. In single crystals with cubic symmetry of properties, especially if the direction of one of the coordinate axes coincides with the diagonal of the cube plane—the direction [011] of the single crystal, in some planes negative values of Poisson's ratios (auxeticity) appear, and also Poisson's ratios greater than 0.5 and even more 1. The paper is presented the results of numerical simulation of the Taylor test: the impact of a cylinder made of a single crystal alloy VZhM8 over an undeformable target with an initial velocity of 50 m/s. All calculations are performed in a three-dimensional formulation using original programs. Various variants of the orientation of the crystallographic axes of the single crystal of the VZhM8 nickel alloy relative to the axis of symmetry of the cylinder are considered. Investigations of wave patterns of deformation in the cylinder cross sections depending on the orientation of the crystallographic axes of the single crystal of the VZhM8 nickel alloy relative to the axis of symmetry of the cylinder are carried out. Cases of compression of a part of the cylinder adjacent to an undeformable target are shown simultaneously in two directions in the plane (001) up to the moment of the cylinder rebound from the target. The study was carried out at the expense by grant from the Russian Science Foundation (project No. 18-71-00062).

Development of dislocation plasticity model for description of shock wave dynamics

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We present our recent results on atomistic simulation of elementary processes in dislocation system (dynamics and kinetics of dislocations) and using of these results for construction and parametrization of the continuum model of plasticity. Simulation of shock wave dynamics is presented in comparison with experimental results with a special attention to the case of ultra-short shock waves.

Molecular-dynamic simulation of shock-wave compaction of metal nanoparticles

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A molecular-dynamic (MD) simulation of the compaction of metal nanoparticles under the action of a shock pulse of picosecond duration is considered. Such a compression pulse can occur when metals are irradiated with powerful femtosecond laser pulses. The layers of nanoparticles are placed in a container or placed freely on the surface of the sample and retained by adhesion forces. A shock pulse is formed in the substrate, which is a shock wave and the following discharge wave. Under the action of the shock wave, compaction occurs due to strong plastic deformation of the nanoparticles. For the case of nanoparticles in a container, we studied the production of a compact, depending on the amplitude and duration of the shock compression pulse. Depending on the parameters of the action, either elastic compression of nanoparticles or their plastic deformation resulting in compaction was observed. It is shown that the impact of high impact pressures leads to an increase in the number of structural defects and to the danger of a sample breaking due to the rapid process of unloading behind the front of the shock wave. MD simulation shows that a rather wide range of parameters (amplitude, duration and number of compression pulses) can be obtained, leading to the compaction of nanoparticles without disrupting the integrity of the sample. The considered method can be generalized for the formation of nanostructured coatings of various compositions. The thickness of the nanocrystalline coating can be locally changed and controlled by the number of active pulses. The work is supported by the Ministry of Science and Higher Education of the Russian Federation, state task No. 3.2510.2017/PP.

Electrodes erosion influence on the interior ballistics of an electrothermal accelerator of macrobodies

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Previously developed mathematical model [1] for the interior ballistics of an electrothermal accelerator (ETA) of macrobodies [2, 3] was modified. The model can be used to predict the projectile velocity for given values of the mass and size of the projectile, the electrodynamic parameters of the capacitive energy storage, and accelerator parameters. The problem of determining the projectile velocity was solved in a hydrodynamic formulation by numerical integration of the equations of motion, the energy conservation equation, and the caloric equation of state. In the case of neglecting the dynamically changing friction coefficient, the calculation results differ considerably from the experimental data, but the model qualitatively describes the physical processes of interior ballistics of the ETA. Electrodes erosion influence was shown. Use of the ETA allows an increase in the average velocity range (2–4 km/s), which is difficult to achieve for traditional gas-dynamic (powder) accelerators and is economically inexpedient when using light-gas guns. These studies have been motivated by the need for adequate modeling of high-velocity impact of micrometeorites and space debris on the structural materials of spacecrafts.

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Study of the liquid-metal drops fragmentation at a steam explosion

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The models of fragmentation of liquid metal droplets in a steam explosion, based on thermal stresses, shock-acoustic effects and explosive boiling of water inside the melt, are analyzed. Experimental installations, the course of experiments and the results of research are described. The samples were heated in levitation mode above the melting temperature with the inductor and then fell into cold water. The diversity of the forms of the fragments formed confirms the assumption of the existence of various fragmentation mechanisms. Numerical estimates show that the cooling rate of particles during fragmentation can reach 10^9–10^{10} K/s. This is quite enough to produce amorphous alloys. It was found that when a steel drop is heated in air, intense sparking (drop erosion) of the metal is observed, which impedes the film boiling mode of the coolant and helps prevent the explosive fragmentation of the melt. Experiments with solid metal samples to study the process of contact of water with a hot (170–620 °C) surface are described. It has been established that a short (several ms) process, with intense wave generation at the vapor–liquid interface, precedes boiling up of a cooler on a hot surface. This process reduces the temperature of the hot wall and allows the shock-wave theory of droplet fragmentation (pressure pulses are generated during the collapse of steam bubbles) to explain the fine fragmentation of a melt of strongly heated droplets during a steam explosion.
The present work was supported by the Russian Foundation for Basic Research (project No. 18-08-0149).

Shock wave propagation through suspension of metallic particles in liquid

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The research of strong shock wave (over 10 GPa) interaction with a heterogeneous medium is conducted. The medium is the fluid with suspended liquid metallic particles of 1 μm diameter without regard for strength. The present work considers the more complex problem statement of [1], where relaxation effects after shock wave propagation through regular structure of metallic inclusions are investigated. Here we consider arbitrary structure of the inclusions and demonstrate mixture zone behind the propagating shock wave front. Surface tension, physical viscosity and heat conduction are not taken into account.

The mesoscopic smoothed particles hydrodynamics modeling using our massive parallel code CSPH&VD^3 [2] demonstrates strong deformation of the metallic particles. There is no compaction of the included metallic particles in conditions we consider. The phenomenon modelled and the results obtained are important for promising nanotechnologies.

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About a possible mechanism for the formation of hot spots

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This investigation is devoted to the study of the consequences of an initiating shock propagating through a condensed substance on a free surface. To close the laws of conservation of mass, momentum and internal energy, the equation of state of a condensed substance was constructed [1]. The form of this equation of state corresponded to the form of the equation of state of Mie-Gruneisen with the separation of pressure and internal energy into thermal and cold parts [3, 4]. The ratio of the thermal part of the pressure to the thermal part of the internal energy was determined by the Gruneisen coefficient, which in this work was a constant. The cold part of the pressure was described by potential in Theta form. Analysis of the results presented in the work shows that after the shock reaches the free surface, a strong rarefaction wave begins to propagate into the condensed matter, which causes the pressure to drop in the condensed matter and the stress greatly increases, which can lead to a discontinuity of the material and appearance of a separate micro particle. This confirmed the assumption that hot spots could appear as a result of the warming up and burning of the smallest droplets of condensed explosive during the collapse of a gas bubble [4, 5].

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Analysis of the interaction of the spherical shock wave with the forest

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This paper discusses the problem of the interaction of a spherical shock wave with a forest. The results of mathematical modeling of the propagation of a shock wave through a forest are presented on the basis of a two-dimensional system of Euler differential equations in a cylindrical coordinate system [1]. The effect of the disruption of forest combustible materials on the parameters of the shock wave is investigated. It is assumed that the shock wave is formed as a result of the expansion of the spherical volume of compressed hot gas formed after the explosion in the atmosphere of a cosmic body. The distribution of parameters within a given volume is uniform. The forest is modeled by an inhomogeneous layer, the solid phase of which consists of two components (stationary trunks and combustible materials of the forest), which gain speed when the shock wave is destroyed. The pressure drop at the front of the shock wave, obtained experimentally [2, 3] during the propagation of a shock wave in pine forests, was taken as the breakage criterion. The numerical simulation was performed using a modified large particle method.

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A continuum model of iron for simulations of plate impacts and spherical shells under explosive compression

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Continuum models of iron and steel are developed to simulate extreme phenomena where materials are subjected to shock compression up to tens of GPa. In these conditions both the elastic-plastic properties and the polymorphic α–ε phase transition in iron are important. The appropriate equation of state for iron is constructed using data referenced in the report [1]. The model for iron is validated using smoothed particles hydrodynamics method on wave profiles obtained in the plate impact experiments [2], where all the observed fatures including the hysteresis effect of the reverse ε–α phase transition are reproduced correctly. The yield strength of constant 0.5 GPa is found to fit well the elastic precursor amplitude. Wave profiles obtained in the experiments [3] during spherical steel shells convergence under explosive compression have similar structure including α–ε phase transition, but the yield strength is shown to be higher than one for iron.

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Computational fluid dynamics simulations of underwater explosions

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In the last century, great progress was made in the hydrodynamics of an explosion, the science of fluid flows under shock-wave loading. This area is concerned primarily with studying underwater explosions (UNDEX). UNDEX refer to the detonation of explosive devices immersed in water.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. Furthermore, in the case of the explosion occurring close to the structure, a high velocity water jet penetrating the gas bubble occurs. Shallow water underwater explosions exhibit very different characteristics from deep UNDEX. Gravity (buoyancy) affects the bubble collapse event, resulting in a reentrant jet that pierces the free surface. Modern CFD tools with new highly efficient numerical schemes applicable for UNDEX simulations were developed and implemented in commercial and open-source software.UNDEX simulations with OpenFOAM and comparison of numerical results with experiments and other numerical simulations are shown.

Superconductivity of shock-wave pressure treated Na–WO_3 mixture

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Mixture of Na and WO_3 with 1 : 1 molar ratio has been subjected to shock-wave pressure of 20 kbar, followed by vacuum encapsulating and quenching of the product to liquid nitrogen. The ac magnetic susceptibility of the samples has revealed metastable superconductivity with $T_c \approx 40$ K. The samples were prepared with applying the flat-type shock-wave pressure setup, described in detail in [1]. The starting material was tablets, 10 mm in diameter and 3 mm thick, prepared of 1 : 1 molar ratio mixture of 99.99%-pure Na and powdered, 7–14 μm grain size, 99.98%-pure WO_3, corresponding to the composition of a stoichiometric tungsten bronze $NaWO_3$. Comparison of the ac susceptibility measured at different magnetic fields and frequencies infers that the superconductivity arises within the weakly linked superconducting regions formed during the shock-wave pressure treatment. The ac magnetic susceptibility of the produced samples has revealed metastable superconductivity of $T_c = 40$ K. Analysis of the experimental data infers that the superconducting phase consists of the weakly linked regions, which are embedded into a non-superconducting host matrix consisting of the Na_2WO_4, $Na_2W_2O_7$, WO_3 and metallic W phases.

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Effect of mechanical activation on combustion characteristics of Al–CuO powder mixture

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The practical use of exothermic chemical reaction in the form of the combustion may be associated with one or another of its manifestations. Such a manifestation can be the mass flow, heat release power, quality and intensity of optical radiation, etc. The effectiveness of these manifestations depends on the mixing conditions of the initial components to a large extent. In this paper, the character of manifestations of the chemical reaction of Al–CuO under different conditions of its implementation is investigated. The ultimate goal of the study is to optimize the parameters of mechanoactivation of this mixture for its effective use in various conditions. Before the experiments, the mixture of components was subjected to mechanical activation. The prepared mixture was placed with controlled porosity in experimental assemblies and a chemical reaction was initiated. The parameters of the study were the time of mechanical activation, the porosity of the samples, the method of initiation and the scheme of the experiment. The brightness temperature and the speed of the boundaries of the glow area were the subject of research. High-speed camera, pyrometer, photoelectronic and electrocontact sensors were used as diagnostic tools.

Formation of Bi_2CuO_4 by the self-propagating high-temperature synthesis

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Bi_2CuO_4 is used as high-temperature superconductors precursor in the synthesis of $Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$ from oxides. In our work, an attempt was made to synthesize bismuth cuprate by the self-propagating high-temperature synthesis (SHS). SHS technologies have indisputable advantages, including high performance, low cost price. This technology is well known. To the stoichiometric mixture of solutions of the prepared nitrates it was added an equivalent amount of the feed stock heated to self-ignition: glycine (G), urea (C) or citric acid (L). The burning process is very intense. The phase analysis and the calculation of the coherent scattering region (CSR) of the products were carried out on Shimadzu XRD-7000 x-ray and Rigaku SmartLab diffractometers. Analysis of x-ray diffraction patterns showed that the use of urea for samples with a nitrate ion/reductant ratio of 1 : 1 allows to obtain a sample with only one crystalline phase (Bi_2O_3 tetragonal modification). If L or G were used, a multiphase sample was synthesized, in which, along with bismuth oxide (Bi of the rhombic structure) and Cu of the cubic structure were identified. It has been established that the type of feed stock influences the average size of the CSR phases. Thus, the samples synthesized using urea have a minimum CSR size: Bi_2O_3 15–20 nm. In addition, it was found that only when citric acid is used monoclinic modification of Bi_2O_3 is present, and C and L are used tetragonal modification of Bi_2O_3 is obtained.

Study of the kinetics of chemical interaction in ignition of thermite-type compositions

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The initial kinetics of the chemical interaction of compositions based on aluminum and oxides of some metals is determined. The choice of metal oxides is based on the low value of the heat of their formation. Methods of mass (TGA) and thermal state (DSC) measurements at controlled sample heating were used. The rate of heating was of the samples weighing 5–10 mg were 10 deg/min in argon flow of 100 ml/min. Sample heating to a temperature of 600±50 °C leads to the beginning of the exothermic heat release up to the melting temperature of aluminum particles. The melting of aluminum particles blocks the fixation of the exothermic nature of the interaction. Fixation of exothermic heat is resumed after the melting of aluminum is completed. The secondary exothermic heat release is due to the activization of decomposition of metal oxides with increasing temperature, apparently. The rate of exothermic release for the studied compositions ranges from 200 to 1000 J/g. Heat generation was stopping when the sample substance burns out. The author is grateful to N Muravyov, A Pivkina, K Monogarov and D Meerov. The work was performed on the equipment of the Laboratory of Energy Materials of the Institute of Chemical Physics RAS.

The formation of a detonation wave with multipoint initiation

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The solution of many practical and scientific problems using explosives requires the use of detonation waves of various shapes (cylindrical, plane, conical, spherical, etc). One of the simplest methods for generating such waves is the multipoint initiation method. In previous works, the authors showed the presence of a rather complex structure of such a wave. The causes of the formation of such a shape and the ways of smoothing its complex volume-cellular structure were determined, since it is the cause of many undesirable phenomena. These include hydrodynamic perturbations on the surface of a compressible liner, the ejection of plasma and material particles into the volume under study, and others. In this paper, it is proposed to use special shaped shapes for the points of initiation. These forms are made of polymer on a three-dimensional (3D) printer and filled with explosives. In this case, the initial stage of interaction of detonation waves from neighboring points occurs in charge at lower angles. This significantly reduces the intensity of such conjugation of waves. Another way is to form a section of a cylindrical wave with inverse curvature. For this purpose, specially shaped lenses made of inert material are used, which are located between the surface of the main charge and the points of initiation. Preliminary calculations of such a lens have been carried out, its three-dimensional model has been built. A prototype is made of polymer material on a 3D printer. Experimental results for cylindrical and plane detonation waves formed by the multipoint initiation method using polymer elements are presented.

A magnetic-cumulative generator with open switch unit

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Experiments with magnetocumulative generators were conducted for model inductive loades 5 μH. The generators were designed and investigated with a primary circuit being switched off. An explosive open switch ensured a voltage front pulse in the loads, with the pulse leading edge no more than 4 μs. Intercepted magnetic flux in a primary circuit was 0.08 Wb, and output electrical parameters were registered: energy 8 kJ, a magnetic flux of 0.3 Wb, coefficient of flux conservation about 0.6. The tests under consideration have demonstrated a high performance and effective application of the small-sized devices for impulse magnets supply.

The role of gas flame instability mechanisms in its acceleration

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To study the role of individual mechanisms of instability of the flame front, a series of experiments was carried out on the propagation of a spherical flame. Transparent latex shells were filled with pre-prepared hydrogen-air mixture. In various series of experiments, the percentage of hydrogen was varied. The ignition of the flame was produced by a spark discharge with an energy of 1 mJ, a discharger located in the center of the shell. Experimentally, the scattering parameters of the spherical hydrogen-air flame acceleration was found with a constant mixture composition and combustion initiation energy. It was found that at the initial stage of propagation, both acceleration and deceleration of flame front occurs. The parameters of the flame front propagation experimentally obtained are supplemented by calculations carried out using analytical models. The values of the growth rate by various mechanisms of instability and the size of heterogeneity at which the main growth mechanism is changed are calculated.

Control of instability of the flame with heat losses

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The smooth flame front in the premixed fuel mixture is unstable. The consequence of this instability is the curvature and acceleration of the flame front. This leads to a regime of rapid combustion, deflagration and detonation. The scale and growth rate of the flame front instability are determined by the properties of the combustible mixture, the kinetics and thermodynamics of the chemical reaction. The impact on any of these components of the combustion process allows to change the parameters of the flame front, and, consequently, its acceleration.

This paper presents an experimental investigation of the propagation of hydrogen–air flame with heat loss. The influence of heat losses on the expansion of combustion products and the density of the flame surface is analyzed. It is shown that the removal of part of the heat released during combustion can significantly affect the number and nature of inhomogeneities on the surface of the flame front, reduce the flame propagation velocity and suppress the acceleration of the flame front. The topic and results of the study are crucial in the areas of internal combustion engines, detonation initiation and explosion safety issues.

Experimental study of shock wave reflection from porous materials

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The development of methods for attenuating shock waves with the use of porous materials is an urgent scientific and practical task, the solution of which is devoted to many studies. It was found that the maximum pressure in the final phase of the interaction of direct and reflected shock waves with a porous material exceeds the pressure behind the shock wave of the same intensity reflected from a free solid surface. This anomalous growth was due to the effect of deforming porous material on the pressure sensor. No detailed explanation was given for the additional increase in pressure behind the shock wave reflected from the porous material.
We have supposed that the process of interaction of a shock wave with a porous material is affected by five factors: the permeability of the material, its elasticity, density, sample thickness and intensity of the primary shock wave. Therefore, in the present work, the interaction of shock waves with foam density and steel wool was investigated. The experiments were carried out in a shock tube with Mach numbers M = 1.1–1.7. Samples were installed close to the end wall of the low-pressure chamber. Pressure measurements were carried out with four piezoelectric sensors. In some experiments, the free surface of the samples was covered with a thin film of scotch to eliminate the effect of permeability of the material. The results of the experiments allowed us to identify the features of the interference of shock waves and sound compression waves during the interaction of the primary shock wave with various porous materials.

Detonation property of gelled liquid explosives based on nitromethane plus ammonium perchlorate mixtures

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Experimental results on detonation properties of gel-like explosives (LE) based on heterogeneous thickened nitromethane (NM) plus ammonium perchlorate (AP) particles mixtures are represented. The objective of the experiments was to assess detonability and detonation parameters of these mixtures at various initial conditions. Detonation velocity was measured versus gelling agent concentration, AP particle size, mixture richness and tube internal diameter. The results of critical diameter measurements and heat explosion safety tests results is also represented. Such type of LE is very promised to be used in practice as explosive component of explosive proppants capable of detonating in narrow cracks or proppant pores and intended to be used for far field fracture stimulation of oil bearing formation subjected to hydraulic fracturing. Introduction of inert microparticles in NM is known to increase its sensitivity to impacts and reduces the critical charge diameter. Some more recent data demonstrate reduction of the critical detonation diameter of NM mixed with AP particles. A comparison of the results of tests performed led to an unexpected result. Detonation velocities of mixtures with coarse AP particles are higher than with fine ones. Critical diameters experiments demonstrated that it increases monotonically as the mixture gets richer and the AP particle size increases. Heat explosion tests demonstrates that as the equivalence ratio increases the thermal explosion temperature decreases. Experiments represented clearly demonstrates a possibility of using the mixtures studied as part of explosive proppants.

Slurry nitromethane plus ammonium perchlorate mixtures infilled into the inert matrix of the ceramic grains as explosive proppant

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The object of the study is liquid or gel-like explosives (LE) capable of detonating in narrow cracks or proppant pores and intended to be used for far field fracture stimulation of oil bearing formation subjected to hydraulic fracturing (HF). LE is based on heterogeneous thickened nitromethane (NM) plus ammonium perchlorate (AP) particles mixtures. The objective of the work is to assess as detonability of such mixtures infilled into the inert proppant matrix of various porosity, as to clarify the possibility of application in HF by demonstration of explosion in convergent narrow crack in concrete block filled with explosive proppant. Experimental results on detonation velocity of LE-proppant mixtures in tubes of various internal diameters are discussed. Results of experimental comparison of detonability of LE studied with pure NM in proppant matrix also represented. The goal of the present work is to demonstrate applicability of LE in rock fracturing.

Study of detonation-like mode of destruction in silica fiber under laser action

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Damage of the light conductivity in the fiber waveguide transporting intense laser radiation leads to the absorption of energy and the appearance of a bright laser plasma. The plasma begins to move towards the radiation source, damaging the light guide. Depending on external laser energy, different damage propagation velocities are possible [1, 2]. In any propagation mode, the damages of core are irreversible. The diameter of the studied laser plasma was 7 μm.
The developed experimental techniques let us to visualize the structure of the detonation front in silica based fibers under the intense laser action [3, 4]. It was shown the pressure wave front has complicated structure.
This work has been done due to support of basic research program of the Presidium RAS (I.31P).

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Dynamics of supersonic waves of spin reversal in molecular magnets

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We investigate the dynamics of supersonic waves of spin reversal in molecular magnets within continuum framework, generalizing the stationary model introduced in [1] to include non-stationary effects. The theory is based on the reactive Euler equations with a non-ideal equation of state, wherein the reaction is that of exothermic spin reversal releasing the Zeeman energy of spin states in an external magnetic field. The forced Burgers equation is derived asymptotically, which seems to have much in common with the nonlocal toy model of detonation in [2] and the asymptotic model in [3]. We discover that the solutions of the model in the form of traveling shock waves can become unstable when the magnet's initial temperature and the strength of the imposed external magnetic field are sufficiently low. Beyond the stability threshold, the wave dynamics is found to be either periodic or irregular.
This is a joint work with Luiz M Faria (INRIA, France) and Rodolfo R Rosales (MIT, USA).

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Explosive crystallization in thin film ferroelectric precursor by strong femtosecond pulse

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Explosive crystallization of local ferroelectric microstructures was investigated experimentally and was described by theoretical model which takes into account a release of crystallization latent heat on the crystallization front and thermo-induced mechanic stresses which increase crystallization activation energy [1, 2]. Strong near infrared femtosecond laser source was used for local heating. Our estimations give value of integral laser intensity from 1.3 to 1.5 MW/cm^2 which provides crystallization. Such a strong thermal effect led to the appearance of periodic film detachments from the substrate. Heat source in structures $Pb(Zr,Ti)O_3/Pt/SiO_2/Si$ was located in platinum sublayer as ferroelectric precursor thin film is transparent for laser beam. Theoretical model explains why crystallization starts on the precursor surface instead of heat source (it was observed by transmission electron microscopy of microstructures cross-sections). Nonlinear-optical microscopy was used as main technique for studying local ferroelectric microstructures. One can obtain different types of microstructures: local circle structures, local ring structures and microwaveguides. Latter is possible due to refraction index of annealed area is higher than of non-annealed surrounding. Such microwaveguides can be used for short distance light transfer between optical elements. By such technique it is also possible to create 1D and 2D nonlinear photonic crystals.

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Destruction of crystal structure of detonation nanodiamonds under thermal heating and irradiation

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Thermal and radiation effects modify particles of detonation nanodiamonds. Irradiation damages the crystal lattice. These injuries vary depending on the energy, type and dose of radiation. Point defects, amorphous phase and graphite phase are formed in the diamond volume [1]. Annealing of irradiated samples with point defects leads to the release of stored energy and restoration of the lattice. The high energy ions can modify internal part of nanodiamond core. The heat treatment of detonation nanodiamond in inert dynamic atmosphere leads to destruction of crystal diamond structure beginning with its surface [2]. The detonation nanodiamond (DND) is stable up to 500 °C. Beginning at 600 °C, the diamond phase slightly decreases. Nanodiamond transition to amorphous phase was assumed. Some part of nanodiamonds were stable to heating up to 1500 °C [3]. In the normal state, the DND is a powder of conglomerates of individual nanodiamond grains. It was found that the size changing of conglomerates depends on heat treatment rate.

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Detonation properties of the tetranitromethane–methanol mixture

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A chemical reaction in shock-compressed liquid high explosives (HE) has a thermal character, and initial rate of reaction is a strong function of activation energy. It can change in a wide range by addition of diluents to HE. Definition of the initial rate value gives important information for prediction of HE detonation due to its influence on the detonation wave structure and propagation limits. In this work, the reaction zone structure, stability of detonation waves and limits of detonation propagation in the tetranitromethane–methanol (TNM–M) mixture, depending on the diluent concentration, were investigated by VISAR interferometer. In the experiments, on the dependence of particle velocity on time, in the neat TNM behind the shock jump the velocity decreases smoothly and the maximum velocity gradient is realized directly behind the shock wave front. At the addition of methanol to TNM, the amplitude of Von Neumann spike begins to decrease, whereas detonation parameters increase. At the methanol concentration of 15%–35%, there is a sharp change in the character of the reaction zone–after the initial shock jump, the particle velocity continues to increase, for approximately 10 ns, reaches maximum, and then drops. At the increase of methanol concentration from 40% to the critical concentration of detonation (60%), the detonation parameters decrease and oscillations appear on the velocity profiles. It means that detonation front becomes unstable. The dependence of detonation velocity of the mixture on methanol concentration is non-monotonically. The highest detonation velocity is observed at a small negative oxygen balance (about 26%–28% of methanol). This work was supported by the Russian Foundation for Basic Research (project No. 16-29-01002).

Research of the beginning of spherical detonation of hydrogen–air mixtures under direct initiation near the critical point

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Investigation of the detonation of hydrogen–air mixtures is of great importance for the gas dynamics of combustion and for the safety of nuclear power plants and other facilities using hydrogen. We studied a development of spherical detonation at its direct initiation. In this study, the hydrogen-air mixture was placed in a thin rubber envelope with volume of 7 m^3, having a shape close to spherical, which was located into the explosion chamber 13Ya3 with inner diameter 12 m. After filling, the mixture was blended by a fan for 30 min, then the fan was turned off, and the mixture was being aged for some 30 min to level the composition further.

There was a measuring bar inside the envelope at which pulse pressure sensors, measuring the pressure in the front of the detonation wave, and ionization sensors, detecting the movement of the flame front, were placed. The mixture was ignited in the center of reaction volume. The initiation energy was equal to 4.6 kJ that was achieved by explosion of 0.4 g PETN charges. In the present work, we investigated the beginning of spherical detonation in hydrogen-air mixtures with a hydrogen content of 32 to 42 vol %. When the hydrogen content was 32 and 42 vol % detonation did not occur, and at 34, 36, 38 and 40 vol %, it did occur. It has been shown for the first time that spherical detonation of hydrogen-air mixtures occurs when initiation energy is equal to 4.6 kJ. It is revealed that the critical initiation energy (the minimum initiation energy at which spherical detonation occurs) is less than the previously recognized (7.8 kJ).

Damped oscillating combustion in acetylene–air mixtures

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Characteristically, the propagation of detonation in subcritical narrow channels is accompanied by rotation or jumps in the propagation modes. 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 [1, 2]. The relevance of the research on the combustion of acetylene is determined by the energy and environmental interests in this fuel. Given the additional combustion of pyrolysis products, the total energy release can increase up to two times [3].

This work is devoted to a series of experimental investigations of the decaying oscillating mode of the flame propagation for acetylene–air mixture, when the average velocity is significantly lower than the velocity of the stable Chapman–Jouguet detonation. The aim of the work was to determine a criteria for the decaying flame propagation in the acetylene–air mixture, as well as for the galloping detonation propagation.

Experiments were carried out using channels of square cross-section with transverse dimensions of 3×3 and 5×5 mm^2. High speed schlieren image sequences of the reaction zone and shock waves were obtained. Depending on the quantitative value of this parameter, the conditions for the stationary detonation ($D/\lambda = 0.9$–1.0), galloping ($D/\lambda = 1.1$) or damped oscillating combustion ($D/\lambda = 0.4$–0.9) were determined.

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The flame existence limits in channels with narrowing

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The movement of the flame along the channel with a narrowing in the middle is considered. The diameter of the channel is assumed to be sufficient for the existence of a flame everywhere, except for the middle zone. The goal of the study is to determine how small this narrowing can be so that the flame can still pass through it. The relevance of the study is due to the development of micro combustion. This research enriches the fundamental knowledge in micro combustion due to the fact that 2D effects are taken into account. In addition to fundamental knowledge, the considered problem may have applications in fire safety and for objects where it is necessary to prevent the flame propagation. The study revealed that the flame might pass through the narrow zones, which diameters are substantially less than the critical diameter for the given mixture. In addition, the narrowing noticeably accelerates the flame. Flame is stretched and the temperature at the leading point of the flame is increased due the reduction of the interaction time between flame and the cold channel walls. There is so-called the flame "inertia" effect, when the minimal flame velocity is achieved not in the narrowest zone but slightly downstream [1]. This effect also contributes to the decreasing of minimal channel diameter, which the flame is able to pass through. It can be concluded that the fire safety criteria based on the critical diameter is not enough if we consider the channel with a narrowing. It is shown that the cold channel walls do not allow the flame to stretch significantly. Flame stretches much more in channels with walls that can be heated, but the stretch effect is not as much influence on flame extinction as heat losses.

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Three-dimensional evolution of the ultra-lean flame ball under terrestrial gravity conditions

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Near range flames pose a serious problem for fire safety applications. Despite the fact that a large amount of experimental data has been obtained for an ultralight flame under microgravity conditions, for practical purposes it is necessary to study the ultrafine structure in the presence of terrestrial gravity and the associated convective motion. In this paper, results of the detailed three-dimensional numerical modeling of ultra-lean hydrogen-air flame ball development in terrestrial gravity conditions are presented. Three-dimensional structure of the flame kernel is studied and different stages of the flame evolution are identified and analyzed. Obtained results are compared with those previously obtained in two-dimensional calculations [1] that allowed to reveal purely three-dimensional effects in the overall flame development. Thus, the rising velocity of the flame kernel obtained in two-dimensional case appears to be 1.5 times lower than in three-dimensional one due to the proportionality of the buoyancy force exerted on the rising kernel and the ratio of the flame surface to its volume. However, curvature radius near the highest point of the flame surface remains almost the same independent of space dimensionality. Herewith, flame stretch values are also equal that results in similar dynamics of the rising flame kernel involving kernel breakup, secondary kernels formation and their non steady propagation in thermal wake behind the main flame kernel.
Current research was financially supported by Russian Academy of Sciences Fundamental Research Program No. I.2.27.

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The gravity influence on methane–air V-flame stabilization

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The study of combustion processes is important for both the fundamental and applied fields. The gravitational effect on flame characteristics, especially in the field of stabilization, is an important modern task. The instability of combustion from a practical point of view is related to stabilization problems in various technical equipments, such as gas turbine combustors, industrial furnaces, afterburners, etc. One of the applied tasks of stabilizing combustion is to expand the ignition (flammability limits) and stable combustion existence domains (blow-off and flash-back limits) in terms of flow velocity and the fuel equivalence ratio. The present work is devoted to the study of the gravity effect on the methane–air V-flame characteristics and blow-off limits. Such geometry flame features were experimentally investigated under normal and reversed gravity conditions (direction of the flow velocity was changed with respect to the gravitational vector direction).

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Parametric study of the combustion acceleration in lean air–C_3H_8 mixtures activated by nonequilibrium discharge

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Contemporary requirements for internal combustion engines lead to the development of low temperature combustion strategies, and it is considered more effective using a homogeneous charge compression ignition engine. Nevertheless, it is hard to ignite lean mixtures with compression only. It was established [2] that preliminary treatment of fuel–air mixture with non-equilibrium discharge could significantly reduce the ignition delay time for different hydrocarbon fuels. In the previous works (e.g., [3]), authors show that discharge treatment mainly affects combustion because of appearance of chemically active particles. In this work authors further investigate the discharge effect on the ignition of fuel–air mixture by means of numerical simulation of combustion wave propagation. Using one-dimensional numerical simulation authors performed a parametric study under the conditions of the compression engine operating cycle. The dependence of combustion process on several parameters (discharge deposited energy, time of discharge initiation etc) is investigated. The specific chemical kinetics mechanism of ignition acceleration due to discharge treatment is discussed. This work was supported by grants from the laboratory "Kinetics and Physics of pulsed Plasmas and their Afterglow" and the Russian Foundation for Basic Research No. 17-53-16003 and 17-53-16002 (France–Russia).

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Modelling of chemical kinetics of combustion: Detailed versus reduced mechanisms

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Usually, for modeling of chemical kinetics for computation of combustion processes reaction mechanisms with many species have been constantly developed [1]. High dimensionality and stiffness of mathematical models because of non-linearity of elementary reaction rates complicates the numerical integration. It requires large memory storage and high resolution in time and space. In order to run simulations in a reasonable central processing unit time, reduced kinetic models are needed [2]. One of promising approaches to cope with this problem is the so-called flamelets approach [3]. This is based on the assumption about one-dimensional flame structure. However, when it is used in strong turbulent strictly unsteady combustion regimes it may lead to ambiguous results. In the suggested study the method, avoiding difficulties and drawbacks of standard approaches to perform model reduction, is introduced. The suggested approach is the reaction–diffusion–manifold method [4]. It is based on singular perturbations and invariant manifold methods which make it very efficient and attractive for applications. In addition, a detailed implementation strategy for reducing the model is presented and discussed. The approach is illustrated by perturbed laminar flames. The flame structure of the accelerating flame by using detailed and reduced models is studied and compared.

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Thermal effects near particle at supersonic combustible flow

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Explosion study of hydrogen containing mixtures is the basis of safe operation of different plants, including for example nuclear plants, coal mines, flour milling etc. The presence of particles of different nature in combustible mixtures can change the explosion initiating conditions [1]. In our early work [2, 3], the results of simulation of shock detonation initiation at presence of single particle are reported. It was numerically shown that the particle can effectively acts on detonation initiation with widening of detonation limits. In present work in addition to early works the particle is not supposed to be adiabatic and can withdraw heat from supersonic combustible flow due to thermal conductivity. This estimation can simulate broadened range of particle materials.

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Chemical inhibition of the processes of ignition of gaseous fuels

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The problem of the safety of industrial facilities working with combustible substances is becoming increasingly serious. The history of the use of various chemically active inhibitory additives to prevent fire began a long time ago. The introduction of the inhibitor should initiate the capture reaction of the most active radicals that initiate the development of chain reactions of ignition. When igniting a hydrogen-air mixture, such radicals are hydrogen atoms, oxygen atoms and the OH radical. And the introduction of an inhibiting additive initiates reactions linking these radicals to form other, much less chemically active compounds. The purpose of this work was to investigate the kinetics of the interaction of various halogen-carbon with various combustible mixtures under different ignition conditions by the direct experimental study and, based on these results, to analyze the effectiveness and limits of applicability of various halogen-carbon inhibitors. In result of research, it was shown that the difference in the effects of halogen-alkanes on ignition by the method of initiating combustion with a spark and the shock wave method is determined by the strong difference between the following factors: concentrations of active intermediate particles in the initial mixture, gas heating process and temperature range. This work was supported by the Presidium of Russian Academy of Sciences the Program No. 13 “Condensed matter and plasma at high energy densities”.

The promotion of detonation wave of condensation in acetylene by methane additions

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In previous works, the authors proposed the possibility of developing environmentally friendly power plants based on detonation pyrolysis of acetylene. Acetylene decomposition is a highly exothermic process with the release of energy: $C_2H_2 \rightarrow 2C + H_2$ (+227 kJ/mol). The products of this process are molecular hydrogen and carbon black, both are widely used in industry.The main method of acetylene production is the partial oxidation of methane. Unlike acetylene, complete pyrolysis of methane to carbon black and hydrogen is an endothermic process: $CH_4 \rightarrow C + 2H_2$ (−75 kJ/mol). Therefore, this process is very difficult and requires quite high temperatures. It is well-known that under conditions of shock-wave pyrolysis of methane in contrast to acetylene, the process of formation of condensed carbon is practically not proceeding. Therefore, it was considered that an addition of methane to acetylene should inhibit the formation of condensed carbon and suppress the formation of a detonation wave of condensation. However, the unexpected promotion of the process of carbon condensation with the addition of methane in the shock-wave pyrolysis of acetylene was recently discovered experimentally for the first time. This effect is of great practical importance, both from the point of view of the explosion-safety of acetylene and creating power plants based on acetylene condensation. An analysis of the gas kinetic stages of the decomposition of acetylene with the addition of methane showed a significant increase in the rate of pyrene formation, followed by the growth of polycyclic aromatic hydrocarbons due to the efficient formation of propargyl C_3H_3. This work was supported by the Presidium of the Russian Academy of Sciences, program No. 13 “Condensed matter and plasma at high energy densities”.

Experimental study of influence of combustion inhibitors on non-equilibrium uv radiation at hydrogen–oxygen and methane–oxygen mixtures ignition

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The goal of this study was the experimental investigation of the uv radiation of electronically non-equilibrium radicals and molecules, formed at ignition of hydrogen and methane with halogenated hydrocarbons additions behind shock waves. The search for new inhibitors and promoters for the control of the ignition is of interest [1]. It was found that by adding an inhibitors to a hydrogen–oxygen mixture highly diluted in argon (1% $2H_2/O_2$), an effect of promotion of ignition arises (at temperatures above 1200 K for CCl_4 and 1500 K for $C_2F_4Br_2$), in contrast to 10% mixture $2H_2$–O_2, where the additives play the role of strong inhibitors. It is assumed that with increasing temperature, the inhibiting additive decomposes and initiates the formation of active radicals. In a mixture of 10% CH_4–$2O_2$ diluted in argon the 1%–2% of additives play the role of promoters, since high temperatures are necessary for the ignition of methane. The non-equilibrium uv radiation was detected in the range of the wavelengths 220–411 nm. It was found that all additives (CO_2, $C_2F_4Br_2$, CCl_4) result in a significant increase of radiation as in hydrogen as well as methane ignition in all observed spectral ranges (except the OH* line near 306 nm)regardless of the effect on the ignition delay time: inhibition or promotion.This work was supported by the Presidium RAS (program No. 13).

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C_3F_7I dissociation kinetics: Direct experimental study and quantum-chemical calculations

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Currently, halogenated hydrocarbons are widely used in various industries to increase explosion safety. Among the most promising additives, iodine-containing halogenated hydrocarbons, including C_3F_7I, are of current interest. The C_3F_7I molecule is completely ozone-friendly and non-toxic for humans. Nevertheless, for possible industrial application, it is first necessary to investigate the kinetics of its initial dissociation. The $C_3F_7I + Ar \rightarrow C_3F_7 + I + Ar$ reaction at the temperatures 800–1200 K and pressures 0.6–8.3 bar behind incident and reflected shock waves using the atomic resonance absorption spectroscopy technique on a resonant line of I-atom at 183.04 nm have been studied. The initial concentration of C_3F_7I in Ar was varied from 0.13 to 10 ppm. As a result, the first direct experimental data on the thermal unimolecular decomposition of n-C_3F_7I were obtained. Time profiles of iodine atom concentration were used to determine the rate constant temperature dependences and its activation energy. It was found that the obtained values of the rate constant at temperatures below 950 K are close to the high-pressure limit. However, the influence of pressure on the rate constant at elevated temperatures remains noticeable. Experimental data were correlated with the results of the Rice–Ramsperger–Kassel–Marcus master equation analysis based on density functional theory calculations. The low- and high-pressure limiting rate coefficients were obtained over the temperature range $T = 300$–3000 K.

Damping and oscillating of detonation wave of condensation

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In a number of past publications by the authors [1–3], a new physical phenomenon has been described and investigated–the formation of a detonation wave initiated by the energy release during condensation of carbon nanoparticles. One of the important features of this phenomenon, in contrast to the usual detonation wave, is that the condensation rate cannot grow continuously with increasing temperature. At approaching the temperatures of evaporation (or sublimation) of carbon nanoparticles the reversal process of their disintegration begins and condensation rate inevitably has to fall. In work [3], the specific regime of development of the detonation wave of condensation was mentioned, in which the temperature behind the wave was above 2800 K that is close to the sublimation temperature of carbon nanoparticles. In this case, the rate of condensation decreases, which leads to a slowing down of the detonation wave. This work was supported by the Presidium of the Russian Academy of Sciences, program No. 13 "Condensed matter and plasma at high energy densities".

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[2] Emelianov A, Eremin A and Fortov V 2009 *Phys. Rev. E* **79** 035303
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Atomic resonance absorption spectroscopy study of dimethyl ether reactions with atomic oxygen behind shock waves

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Biofuels produced from renewable sources, including ethers and alcohols containing from 1 to 5 or even more carbon atoms, are considered the most promising fuel. Most of the published rate constants for reactions of interaction between biofuels and oxygen are measured in the low-temperature region (300–500 K). However, their use for the actual combustion temperature can lead to significant errors. Therefore, the direct measurements of the rate constants for the reactions between biofuels and oxygen in a high-temperature (900–1500 K) range are an urgent task. The appearance and consumption of O atoms during the reaction of dimethyl ether (DME) and oxygen at temperature of 1600–2300 K and pressures of 200–300 kPa behind reflected shock waves using the method of atomic resonance absorption spectroscopy on O atom resonant line at 130.5 nm have been studied. The mixtures of 10 ppm $N_2O + 10^{-1}$ ppm $(CH_3)_2O + Ar$ have been investigated. As source of O atoms for reaction with DME a nitrous oxide was used, dissociation of which into an O atom and a N_2 molecule is considerable already at the temperatures above 900 K, when the thermal dissociation of DME does not yet take place. As a result, the temperature dependence of the rate constant of the reactions of DME with oxygen was obtained. Obtained data are analyzed and compared with the results of kinetic modeling performed using the Chemkin package. This study is supported by the Russian Foundation for Basic Research grant No. 17-08-01303.

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

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Butanol is a renewable source of energy and in recent years a lot of work has been given to the to the development of chemical kinetic mechanism of combustion of this fuel. The main objective of this research was the experimental study of the interaction between butanol and oxygen at the high temperatures. In the work, the kinetics of reaction of n-C_4H_9OH with O-atoms behind reflected shock waves was studied. As a source for O-atoms the molecules of N_2O were used. The quantitative measurements of the time profiles of concentration of O-atoms were carried out using method of atomic resonance absorption spectroscopy (ARAS) on resonance vacuum-uv line of O-atom at 130.5 nm. The time profiles of the appearance and consumption of O-atoms during the reaction of butanol with oxygen in mixture of 10 ppm N_2O + 10–1 ppm n-C_4H_9OH + Ar at 1600–2400 K and 2–3 bar have been recorded. The comparison of the experimental and theoretical concentration profiles shows some inconsistency of the data. It was suggested that nitrous oxide could interact with butanol at temperatures of about 1000 K before the beginning of the decomposition of these components. Based on this assumption the existing kinetic schemes were supplemented by the reactions of interaction of N_2O with butanol that resulted in satisfactory description of experimental data. The support of this study by grants from the Russian Foundation for Basic Research No. 17-08-01303 and the Presidium RAS is gratefully acknowledged.

Flame flat burner for soot properties measurements

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Soot is a pollutant that has a huge negative effect on air quality, human health and the Earths climate. A better understanding of the soot formation process and the determination of its optical properties are important for optimizing soot mitigation strategies, for increasing accuracy in climate modeling, and for increasing the efficiency of carbon black production. Premixed porous-plug burner flat flames are established as important tools for fundamental combustion research. This flame is designed to maintain a quasi-one-dimensional laminar flow of the fuel–oxidizer mixture. In this flame, the combustion process can be monitored over time by the measurements of kinetic characteristics as function of height above burner. In this study, we have built a premixed porous-plug flat flame burner based on the manufactured McKenna burner equipped with laser-induced incandescence technique for measurements of soot size distribution and soot optical properties. This diagnostic could be applied as along the vertical as horizontal axis of the flame. The results of soot particle sizing and thermocouple flame temperature measurements in dependence on height above burner for sooting ethylene–air flame with equivalence ratio 2.34 are presented. The refractive index function of soot particles at two fixed wavelength 532 and 1064 nm was determined by comparing the results of temperature measurements of laser heated soot with corresponding calculations using known incident laser energy. The variation of refractive index in dependence on soot particle size is discussed. This work was supported by the Presidium of the Russian Academy of Sciences, program No. 13 “Condensed matter and plasma at high energy densities”.

Particle shadow velocimetry technique application for investigation of the characteristics of the fuel spray behind a combustor atomizer under conditions simulating the walls of the flame tube

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This paper is devoted to the droplet size and velocity measurement particle shadow velocimetry (PSV) technique [1] study and application. High-magnification shadow Imaging is very suitable for visualizing particles, droplets and other structures. The technique is based on high resolution imaging with pulsed backlight illumination. This technique is independent of the shape and material (either transparent or opaque) of the particles and allows to investigate a particle size of 7 μm [2]. Particle size, velocity, concentration, shape and distribution, mass flux can be obtained using PSV technique.
The optical scheme adjustment was realized during the work. The experimental investigations of the atomizer fuel spray disperse parameters were carried out under conditions simulating the walls of a combustor flame tube. The comparison with open space atomization measurement results was performed. The results of the two measurements are exactly the same.

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[2] Estevadeordal J and Goss L 2005 *43rd AIAA Aerospace Sciences Meeting and Exhibit, Meeting Papers* 12355–12364

Investigation of quasi-dc discharge influence on fuel jet mixing with supersonic airflow

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We present results of study of quasi-dc electrical discharge for mixing of the fuel jet from a wall-arranged supersonic injector with a wall-normal direction of injection with a supersonic airflow. The location of plasma filament over the fuel jet was achieved by using the nozzle of injector as one of discharge electrodes [1]. Three different gases were tested for simulation of fuel injection: air, CO_2 and C_2H_4. The activation of discharge within all injected gases results in development of fluid instability at fuel–air interface which leads to the mixing enhancement. In this work, the analysis of data, including high-speed schlieren visualization and video recording, particle image velocimetry measurements of velocity field, electrical measurements, and pressure obtained using a Pitot probe, demonstrates that the quasi-dc discharge operation significantly affects the large scale coherent structures generation on the leeward side of the jet and in the jet wake thus improving the mixing of the jet with the airflow. In the case of C_2H_4 injection, the plasma filament dynamics was observed to be especially unstable comparing to the air or CO_2 jets. This fact is explained by the discharge specific localization during the injection of ethylene. Based on spectroscopic measurements, it was shown that, in the case of C_2H_4 injection, the discharge is localized in the jet, whilst, in the case of CO_2 injection, the discharge is localized in the air surrounding the jet. This work is supported by the Russian Foundation for Basic Research, grant No. 18-08-01452.

[1] Savelkin K V, Yarantsev D A, Adamovich I V and Leonov S B 2015 *Combust. Flame* **162** 825–835

Features of the arc discharge propagation in channel of magnetohydrodynamic spark jet actuator

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The paper presents an experimental study of magnetohydrodynamic (MHD) spark jet drive. The tests were carried out in atmospheric air. Plasma radiation was measured in a MHD synthetic jet. A high-speed survey was carried out in the luminous region of the plasma cord during its propagation in the channel. The results were compared with the propagation of the arc channel on the surface of the model with similar electric pulse parameters. It was shown that the velocity of the arc in the channel is significant higher than the velocity of the arc in the surface model. The flow visualization of the jet after a single discharge pulse was performed in a wide variation of the pulse parameters. Evolution of the flow after a single MHD actuator pulse was investigated experimentally by Schlieren photography and particle image velocimetry (PIV). The Schlieren photography shows that the pulse energy input causes a compression wave. It has been found that the maximum velocity of thermal point was about 100 m/s. In other hand, the flow velocity inside the jet in a predetermined configuration may be up to 250 m/s [1]. The PIV visualization allowed to assert that the reverse flow rate of the MHD actuator during the relaxation period after the end of electric pulse is lower than in the classic spark jet actuator. Thus happens due to asymmetric mechanical action. The additional inlet for suction of cold gas can lead to decrease the cavity refilling time. Parametric dependences of the jet velocity on discharge current, pulse duration, and energy deposition were measured.

[1] Kazanskiy P N *et al* 2016 *J. Phys.: Conf. Ser.* **774** 012152

Parametrical investigation of mixing by a spark discharge in supersonic flow

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Previously the spark discharge was discussed as a possible actuator for mixing enhancement in supersonic flow [1]. In this work the results of numerical simulation of a fuel mixing with a supersonic flow by a long spark discharge are presented. The transonic injection of fuel is organized by wall-mounted injector 4 mm diameter, and discharge is located near the wall downstream the injector. Discharge is modelled using volumetric heat source. Parametrical investigation which includes variation of fuel mass flow rate, discharge energy, shape and location was performed with the aim to describe principle view of plasma actuator and limitations of its application to the mixing in the supersonic flow. It was observed that spark discharge improves the mixing of jet with supersonic airflow. The interface between the fuel and oxidizer has a bigger surface in the case of transverse discharge than at using the longitudinal plasma channel. Energy release at one discharge should be about 0.1 J and it is better to locate spark channel 15 mm downstream the injector. Typical repetition frequency of discharge pulses for pulse-periodical mode should be more than 6000 Hz to provide a continuous effect on the mixing.

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Experimental research of heat and mass transfer of laser heated carbon in supersonic flow

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Supersonic and hypersonic vehicles undergo significant overheating during the flight, which can cause damage to the vehicle. Current research is dedicated to the investigation of the interaction of laser heated carbon samples and supersonic flow. For the tests, supersonic wind tunnel was used with flow speed of 520 m/s and Mach number 2 at the nozzle exit. Heating of the surface of samples was provided by infrared laser with emission length about 1070 nm and maximum laser power of 1 kW. Conical sample geometry with cone angle equal to 38° was used for the experiments. Heating duration was in the range of 5–10 s.

The mass loss of the samples was measured; for different structured carbon samples, it varies in the range of an order. For samples with the same structure, a linear dependence of the mass loss on the heating duration was found when the heating duration exceeds 20 s. The results are consistent with a similar study of coals heated in plasma [1], which also revealed the nonlinearity of the mass loss from heating time over short time intervals. The mass losses were also measured by laser heating without supersonic flow. It was found that mass loss without flow is 30% of the mass loss in a supersonic flow.

[1] Tyuftyaev A S, Gadzhiev M K, Sargsyan M A, Chinnov V F, Demirov N A, Kavyrshin D I, Ageev A G and Khromov N A 2016 *J. Phys.: Conf. Ser.* **774** 012204

Numerical and experimental investigation of integral characteristics of cruise hydrogen scramjet demonstrator

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Present-day developments in the field of civil hypersonic aircrafts are carried out in many countries [1]. The most important component of such aircraft is the power propulsion (PP) integrated to the airframe. At such high flight speeds a scramjet, or a combined scramjet PP are usually considered for these purposes. The results of numerical simulation of hydrogen scramjet demonstrator with an under-fuselage engine arrangement with a flat air intake device are presented. The results of experimental tests are given also. The possibility of obtaining of engine thrust which exceed the vehicle drug for the test facility regime the same as for HEXAFLY-INT project [2] is shown.

The work was supported by the Presidium RAS within the scientific program "Condensed matter and plasma at high energy densities".

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Analysis of the effect of boron-containing compounds and combustion catalysts on the paraffin combustion rate in an oxidizer flow

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Today, hybrid rocket engines (HRE) working on solid fuel and liquid or gaseous oxidizer are a promising trend in the rocket engine engineering area, because they have such advantages as draught controllability, high specific impulse, insensitivity to defects in fuel, and simple design. One of the key challenges in HRE development is the creation of high-energy oxygen-free solid fuels with high combustion rate, and provision of their full combustion in a gaseous oxidizer flow. A new trend in the improvement of the characteristics of solid fuels is the utilization of boron-containing compounds as energy-intensive admixtures and organic-metal complex compounds as combustion catalysts.

The tests on the combustion of solid fuel samples based on paraffin in the gaseous oxygen flow have been carried out in ITAM experimental facilities. The tests have been carried out at the atmospheric pressure and oxygen flow velocity of 31–27 m/s. The combustion rate of the solid fuel samples increases when amino-borane, and sodium tetrahydridoborate with a solid oxidizer are added to paraffin.

Application of composition elements in the system of diagnostics of parameters of high-enthalpy flow in cut of aerodynamic nozzle of a high stand

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The basic design features of the installation on an attached air duct, which makes it possible to carry out resource autonomous testing of structural elements made of carbon–carbon composite materials, are shown schematically. Cylindrical tubular samples made of carbon–carbon composite materials were tested under high-enthalpy air flow at a full pressure of up to 5 bar and a temperature of up to 1900 K. The maximum diameter of the samples was 10 mm with a wall thickness of 3 mm and a length of 75 mm.

Experimental dependences of the surface temperature of samples of carbon–carbon composite materials in the regime of flow around a high enthalpy air stream for 300 s were obtained. The efficiency of cylindrical tubular samples of a surface siliconized carbon–carbon composite material has been confirmed. Conclusions about the possibility of using carbon–carbon composite material in the manufacture of thermally loaded structural elements in the system of scanning temperature fields during the operation of high-rise stands with an aerodynamic nozzle are made.

Analysis of the possibility of reducing the gas-dynamic loadings arising during the operation of the liquid-propellant rocket engine by injecting water into an exhaust jet

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The main objective of this work is to estimate the effectiveness of reducing of the gas-dynamic loadings on the launcher by the water injection into the exhaust jet of the liquid-propellant rocket engine. A design model of the launcher was created to study this method conceptually corresponding to the available launch sites and test benches. Water coolant was injected into the exhaust jet in various ways. The discrete phase model method was used to simulate a two-phase medium, the disintegration of the jet and drops was performed using the Kelvin–Helmholtz or Rayleigh–Taylor model [1]. The work was done in two stages. The first one is a calculation performed with water injected in the liquid and gaseous phases into the cross-flow. At the second one, the efficiency of reducing gas-dynamic loadings was evaluated. A comparison of the results of numerical calculation with an analytical solution, which was obtained by the formulas verified in [2, 3], was conducted.

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Influence of vortex generators on autostart of supersonic small-scale input devices

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To present day, there are practically no publications on the influence of vortex generators on the autorun borders of supersonic small-scale intake devices. There are works dedicated to: the separate development of the wake behind the vortex generators, the influence of the vortex wake on the gap caused by the interaction of the jump with the boundary layer, and the influence on the characteristics of supersonic devices in general. In this case, the advantage of vortex generators is the possibility of their use for increasing the autorun boundaries. Note that one of the problems with the use of vortex generators is the difficulty in selecting the shape of the device for flow conditions. For this reason, an example of the selection of the shape of tetrahedral vortex generators on a smooth plate blown by a flow on the Mach number M = 3 is given in the work. The selection of the shape of the device generating the vortices was carried out on the basis of numerical simulation of the flow in the wake behind the vortex generators. Consideration of the influence of vortex generators on the autorun boundaries was carried out on a one-jump input device model. The autorun boundaries of the input device were considered both numerically and experimentally. The results presented in the paper showed a positive effect of vortex generators on the operation of small-scale supersonic devices.

Validation study of hydrogen combustion in a supersonic flow of an oxidizing medium with axisymmetric and plane flow

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When developing high-speed hydrogen combustion chambers, much attention is paid to increasing the efficiency of the organization of mixing the air-fuel mixture. In the case of high-speed flows, when the residence time of the fuel–air mixture in the flow path is small, the combustion efficiency is determined not only by the quality of mixing the components, but also by the mechanisms of chemical kinetics. In this work, the combustion of a hydrogen–air mixture was simulated in the case of an axisymmetric flow in the flow path in the configuration of the Beach–Evans experiment and in the case of a flat flow in the flow path in the configuration of the Burroughs–Kurkov experiment. The influence of the used calculation methods and boundary conditions on the solution of the problem of burning a hydrogen–air mixture in the mixing layer was investigated. Menter and Re turbulence models, the mechanisms of chemical kinetics of Dimitrov, Hanson–Hong, Starik, the pulsating component models of the flamelet, laminar finite-rate and eddy-dissipation concept were used. The inlet turbulence was varied. It is shown that the method of accounting for the pulsation component in determining the concentrations of components has a decisive influence on the quantitative and qualitative character of combustion in the mixing layer. The best agreement with the experimental data was obtained using the flamelet model. The reported study was funded by the Russian Foundation for Basic Research, project No. 18-31-00254.

Numerical simulation of the inertial trap of solid particles under test facility conditions

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A large number of high-temperature environmentally hazardous substances are formed during experimental studies of solid propellant rocket engines. Depending on the chemical composition of the combustion products, water or alkaline can be supplied to the exhaust diffuser to neutralize them. This approach allows not only to reduce the temperature of exhaust gases to the desired value, but also to convert volatile harmful substances into acids (for example, in hydrochloric and boric acid). The task of the inertial trap is to prevent water droplets and condensed particles (c-phase) from entering the atmosphere. Inertial trap in which solid and liquid particles are removed from a swirling flow under the action of centrifugal forces are called cyclones. The higher the velocity at the inlet of the cyclone, the more centrifugal force acts on the particles. However, an increase in cyclone efficiency is detected only up to a certain maximum inlet flow rate, after which cyclone efficiency is reduced. In this work, during the numerical simulation of the test facility cyclone, the distribution of solid particles with a diameter from 1 to 500 m is set at the diffuser entrance. A discrete phase model is used, in which the trajectory of particles or droplets is calculated in the Lagrangian coordinate system. In order to simplify the task, water droplets are considered as solid indivisible particles with a given density. The efficiency of the cyclone is estimated by the ratio of the number of particles trapped in the exhaust diffuser to the number of particles deposited in the cyclone.

Modeling of reciprocating-engine combustion regimes including detonation

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Improving reciprocating engines requires detailed analysis of ignition and flame propagation in the combustion chamber. This paper presents the results of in-cylinder flow computations demonstrating piston motion under various combustion regimes ranging from flame propagation to detonation. Two-dimensional computations are performed by using the Gas Dynamics Tool package for a piston–cylinder assembly using a model mixture at an equivalence ratio corresponding to 35 vol % of hydrogen in air. The cylinder diameter is $D = 100$ mm, and the combustion chamber has a top dead center clearance height of 15 mm. Spark ignition is simulated by introducing a millimeter-sized region of elevated temperature and high pressure at zero spark advance. The combustion regime is changed by varying the initiation-region dimensions so that the reaction front propagation velocity varies between approximately 20 m/s and detonation. An analysis of computed results shows that piston motion depends on combustion regime: the highest acceleration and velocity are observed under detonation conditions. A result of practical importance is that the relative efficiency η of detonating combustion defined as the piston velocity ratio between detonation and flame-propagation conditions strongly depends on piston stroke length S. For $S/D = 0.5$ (short-stroke engine), $\eta = 1.5$. For long-stroke engines, with S/D more than 1, the efficiency is lower, η less than 1.2. These results can be used in optimizing combustion processes for sustainable engine designs.

Numeric research of influence of rotation detonation engine model combustion chamber geometry on its thrust-economical characteristics

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Rotation detonation engine (RDE) is one of alternatives of prospective high-speed aircraft engines. Its significant advantage is a low-length combustion chamber (CC). However, the gas flow in such engine has rather complicated unsteady structure. This factor exerts considerable influence on jet nozzle and, as a consequence, on the RDE thrust. The versions of RDE CC with different central body and walls shapes are considered in this paper. The results of thrust-economical characteristics comparative calculations at the same parameters at CC inlet are given. The tasks are solved in three-dimensional transient formulation. A homogeneous oxygen–hydrogen mixture is supplies from one of the axisymmetric calculation area butts, outlet boundary condition is at the other one. Parameters at the inlet are calculated by means of de Laval micronozzles system with back pressure [1, 2] and are specified on the basis of experimental data from [1]. A detail kinetic mechanism of chemical reactions and one-equation model of turbulence are used in a reacting mixture flow calculation. After flow stabilization in CC axial component of full impulse of flow at its outlet section is calculated. Annular CC of cylindrical geometry, with convergent central body and with divergent external wall are considered.

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Numerical simulation of high-temperature pyrolysis of benzene

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Pyrolysis of benzene is numerically simulated using several detailed chemical mechanisms (DCMs) available from the literature. The computed benzene consumption and product yield are compared with experimental data from shock tubes and flow reactors. Temperature and pressure were varied from 1200 to 2200 K and from 0.5 to 50 bar, respectively. Wide discrepancies are found not only in the experimental data on benzene pyrolysis but also in the results of numerical simulations using different DCMs. The key reaction pathways that dominate the process are analyzed. Reasons are given for the difference in numerical results, and explanations are proposed for discrepancies in experimental studies of high-temperature pyrolysis of benzene. Computations of benzene pyrolysis are performed at lower temperatures ($T < 1200$ K) and $P = 1$ bar, for which no experimental results are available in the literature.

Vortex generation by the single arc in the transversal magnetic field

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Pulsed electric arc filament, generated near the wall in the external magnetic field transversal to the current direction is studied from the position of the gasdynamic disturbances induced in a quiescent air. Analysis is performed based on the experiment and numerical modeling in the two-dimensional magnetohydrodynamics (MHD) approximation. It is shown that after the initial channel is formed and the compression wave leaves the immediate vicinity of the arc, the flow is governed by the Ampere force acting inside the conductive channel. The interaction region at this stage can be divided in two parts: the warm region of the thickness of 2–3 mm with the average temperature of nearly 3 kK and peak one up to 12 kK, where a pair of concentrated vortices is formed, and the surrounding gas.
During the current pulse the arc displacement velocity appears to be nearly constant at the level of 100 m/s at $B = 0.3$ T and $I = 50$ A. After the arc travels a distance of several cavern diameters, the entrainment of the flow towards the wall, created by a "starting vortex", occurs. After the pulse, a single vortex is formed near the wall, with the typical flow velocities in the surrounding cold gas up to 30 m/s. This vortex can be used for the mixing enhancement in the external boundary layer, increasing the convective transport of the momentum and mass towards the wall. Parametric study of the process is fulfilled, with the magnetic field, current amplitude and duration varied. It is shown that the increase of the MHD load parameter $v_x B/E$ leads to the formation of the thinner arc cavern with the higher displacement velocity. The work was supported by the Russian Science Foundation, grant No. 18-19-00740.

Numerical modeling of gasification and combustion of solid fuels in a solid fuel ramjet

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Investigation of solid fuel ramjet performance requires mathematical modeling of gasification and combustion of a solid fuel grain in a turbulent air flow. This report presents such a model of processes inside a solid fuel ramjet combustor. The model is based on Reynolds-averaged Navier–Stokes equations and considers the gas flow inside the solid fuel ramjet combustor, the solid fuel pyrolysis kinetics and the combustion of the gasified fuel. The model is verified by a comparison of the numerical results with the experimental data available from other authors. Dependencies of flow parameters on the solid fuel regression rate and the equivalence ratio were obtained for several types of fuels. The analysis of the numerical results shows an influence of flow properties and thermochemical parameters of the solid fuel employed on combustor parameters.

New insights into the mechanisms of cymatic and self-organized wave patterns excitation for access to the properties of the energetic materials reactionary zones

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Pattern excitation and self-organization are fascinating phenomena commonly observed in diverse types of chemical and physical systems. Both experiments and theory confirm that the micro-scale structures excitation in the energetic materials (EM) reactionary zones is a rather universal phenomenon and their understanding and control can have important implications in technology. In accordance with our concept, the micro-scale structures form both the fractal and self-organized wave patterns in the EM reactionary zones and can be considered as a fingerprints of the unique set of holograms of the reactionary zone. This phenomenon can be understood within framework of universal laws of cymatics. Self-organized wave patterns excitation is one of the keys to access to the properties of the EM reactionary zones: the scale and localization of the induction and energy-releasing areas. Manipulating by self-organization of the micro-scale structures and self-organized wave patterns excitation in the reactionary zones can be provided with use of the system of acoustic waves and electro-magnetic fields, generated by special kind of ring-shaped electric discharges along with resonance laser radiation. Application of special kind of the electric discharges demands the minimum expenses of energy and opens prospects for almost inertia-free control by combustion processes.

Studies of the damping properties of a two-phase mixture of transformer oil with gas bubbles

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In energy facilities that use transformer oil, large-scale accidents are possible if an internal short circuit appears and then develops into an arc discharge. Therefore, in recent years gas-liquid media are of interest due to their damping properties [1], which may be sufficient to prevent the mechanical destruction of the oil-filled equipment during electrical breakdown. For this purpose, an experimental installation was created, where the classical method of electric explosion of a wire is used to study the damping properties of a gas-liquid mixture. Microbubbles with a diameter of 1 mm and 0.5 mm are generated with a tangential gas supply in a narrowing part of the Venturi tube or using a Laskin nozzle, respectively. Registration of the waves of finite amplitude arising from the explosion of a wire is carried out by a sensor based on a U8052 microphone calibrated by a Piezotronics 113B21 PCB pressure sensor. Both sensors are installed coaxially opposite each other at the same distance from the wire. During a wire explosion, the amplitude values of voltage and current are 600 V, 10 kA, and during 15 μs 90 J of energy is released. Studies have shown that when the oil is aerated with a Venturi tube with air bubbles with a diameter of 1 mm, the intensity of the final waves amplitude, decreases almost by 5 times, and when gassing with a Laskin nozzle with bubbles 0.5 mm, the intensity decreases by more than 10 times.

This work was partially supported by the Russian Foundation for Basic Research, grant No. 17-08-00110.

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3. Equations of State for Matter

Neutron stars from the collapse to the merging

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We will consider the current results of observations of neutron stars, including the properties of pulsating superluminous x-ray sources, measurements of the magnetic fields of neutron stars, and the study of the interaction of incident matter with the magnetosphere of a neutron star. Particular attention will be paid to the first detection of fusion of neutron stars.

Constraining equation of state of neutron stars using astrophysical measurements

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Equation of state (EoS) of cold dense matter can be obtained using astrophysical measurements of neutron star (NS) [1]. Precise timing of radio pulsars in binary systems constrained the maximum NS mass to be at least $2M_\odot$, which rules out very soft EoS. Determination of NS radii would narrow down the possible EoS and was a subject of numerous studies. For example, mass-radius relation can be obtained using spectral information on surface thermal emission during x-ray bursts and in quiescent states of NSs in binary systems. Additional constraints come from tidal deformabilities measured using gravitational wave signal from merging NSs. NS parameters can also be measured from the x-ray pulse profiles of accreting, nuclear and radio millisecond pulsars. The latter objects are the main targets for the currently operating NICER instrument onboard of the International Space Station, while the accreting millisecond pulsars are to be observed by the Chinese enhanced x-ray Timing and Polarimetry mission to be launched in 2026. Also measurements of x-ray polarization with the Imaging x-ray Polarimeter Explorer to be launched in 2021 will open a new window to the studies of NS [2]. I will review the current status of the problem, concentrating more on the constraints coming from x-ray bursts and accreting millisecond pulsars.

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Neutron star structure, equation of state, and thermal evolution

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Neutron stars, the most compact stars ever observed, can serve as natural laboratories for studies of matter in extreme conditions. In the cores of the neutron stars, the density can reach $\sim 10^{15}$ g/cm^3, while typical temperatures are of the order of 10^8 K. The measured or estimated magnetic fields of neutron stars vary from $\sim 10^8$ to $\sim 10^{15}$ G, with typical values $\sim 10^{12}$ G. Neutron stars cool via neutrino emission from their crust and core and via heat transport and surface radiation. Spectra of this thermal radiation are formed in thin surface layers with typical temperatures $\sim 10^6$ K. I will review the state of the theory of neutron-star structure, composition, equation of state, and thermal evolution. I will demonstrate the link of the theory of neutron-star thermal evolution to observations of their surface radiation and discuss how it helps us to elucidate the properties of matter in extreme conditions.

Thermodynamics of gaseous plasmas in zero-temperature (vacuum) limit

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Limiting structure of thermodynamic functions of gaseous plasmas is under consideration in the limit of low temperature and density. The remarkable tendency, which was claimed previously [1981 *High Temp.* **19** 494–8], is carried to extreme. In the limit discussed thermal and caloric equations of state obtain almost identical stepped structure when their special forms being exposed depending on electron chemical potential This limiting structure appears within a fixed (negative) range of that is bounded below by value of major ionization potential and above by the value connected with sublimation energy of substance

Binding energies of all possible complexes (atomic, molecular and ionic) are the only quantities that manifest itself in meaningful details of this limiting picture as location and value of every step.

The limiting stepped structure of gaseous zero-Kelvin isotherm is generic prototype of well-known "shell oscillations" in equation of state of gaseous plasmas at low, but finite temperatures and non-idealities. At the same time this limiting form of plasma thermodynamics could be used as a natural basis for rigorous deduction of well-known quasi-chemical approach ("chemical picture") in frames of asymptotic expansion (on temperature, but not density) around this reference system.

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Liquid Rb under high pressure: Electron core ionization

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Alkali metals exhibit unexpected structural and electronic behavior at high pressures. The bcc structure observed at atmospheric pressure transforms into several complex low-symmetric structures with a decrease in coordination numbers. Similar behavior was found for liquid state. Recent studies of liquid Rb have shown transformation of diffraction pattern with the first peak of high symmetry to the appearance of shoulder above 7.5 GPa and to a double peak above 20 GPa [1]. Explanation was given by localization of valence electrons in the interstitials. Another approach to understand these transformations consist in suggesting of the increase of valence electron numbers by overlapping of core electrons with the valence band at strong compression. Double peak for the first diffraction appears for liquid Si and Ge–the elements with 4 valence electrons. To support this suggestion it is necessary to show transformations in the solid state. High pressure phase of Rb above 50 GPa is oC16 similarly to Si and Ge at high pressure [2]. Stability of the oC16 phase was explained within the model of Fermi sphere–Brillouin zone interactions with the 4 valence electrons.

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Vacancions in two-dimensional Wigner crystal

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Of great interest are the correlated quantum systems of many bodies with low density. A recent work [1] presents the low-temperature photoluminescence spectra of two-dimensional electrons (2DES) enclosed in MgZnO/ZnO heterojunctions. The two-dimensional electrons annihilate with the localized valence-band holes. The width of the 2DES photoluminescence band gives the value of the quasiparticle optical density-of-states mass. This value for bulk ZnO changes from 0.6 to 0.3 of the electron mass as the interaction parameter r_s changes from 6.5 to 2.4. The 2DES ground state depends on r_s and may be considered as the electron gas, electron Fermi-liquid ore Wigner crystal. The liquid–solid transition calculations including the effect of impurities gives the transition density $7r_s$ [2]. This allows one to consider the quasiparticles existing in the experiment [1] as quasiparticles in a Wigner crystal. At sufficiently low temperatures, defects in crystals (vacancies or impurities) are considered as quasiparticles and are classified according to the values of the quasimomentum k [3]. The electrons removed from the Wigner crystal are considered as vacancions. The vacancy energy $E(k)$ takes on values inside a strip of width D, which is proportional to the probability of tunneling by the defect. The width D corresponds to the 2DES photoluminescence band [1]. The dependence of band width D on r_s qualitatively coincides with the experimental one. The shape of the photoluminescence band of the Wigner crystal depending on the dispersion $E(k)$, the shape of the experimental line and the shape of the band described by the density-of-states mass are different.

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Equation of state of fluid lead

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For fluid lead a phenomenological equation of state is constructed, which describes with sufficient accuracy its thermodynamic properties in the vicinity of the density driven metal–nonmetal transition. This transition has been recently revealed in the work [1], where thermodynamic functions and electrical resistivity of fluid lead have been measured for a broad vicinity of the transition on the phase diagrame.

The aim of this work is to elucidate the features caused by the metal–nonmetal transition in the thermodynamic functions of the fluid. In the method of constructing the equation of state the experimental fact is essentially used that the isochores plotted in the internal energy–pressure plane are straight lines [1]. It can be shown that the equation of state in this case should have the Mie–Grüneisen form [2]. This equation of state is used to estimate the critical point of lead. A thorough comparison of isentropes obtained from this equation of state with isentropes for unloading shock-compressed lead samples was also made.

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The sound velocity measurements for liquid lead

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We are developing an experimental technique for the measurements of the sound velocity in fluid metals at the high temperatures and pressures attainable in the dynamic experiments [1]. The technique allows one measuring the specific volume, pressure, specific enthalpy and electrical conductivity for a sample during the quasi-static process, in which the volume, enthalpy and pressure monotonically increase from the normal values. To measure the sound velocity, on the sample surface an acoustic disturbance is excited with the use of a laser pulse. The arrival of this disturbance on the opposite surface is detected by a laser interferometer. The sound velocity is determined as the ratio of the measured sample thickness to the time, for which the acoustic disturbance passes through it. Recently, such technique was used to measure the velocity of sound in liquid iron [2]. The present paper reports the measurements results of the sound velocity in liquid lead. The focus is on the improvement of the technique and reliable estimates of the uncertainties of the measurements. Lead is essentially softer material than iron so that the surfaces of the sample sandwiched between the flat sapphire plates can be made sufficiently flat so that the cavities between the sample and the sapphire plates are nearly excluded. The obtained results are compared with the literature data as well as the results of our measurements [1], where the sound velocity values have been determined from the caloric properties of lead. This work is supported by the Presidium RAS within the fundamental research program “Condensed matter and plasma at high energy densities”.

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First-principle description of results of dynamic experiments for refractory metals near the melting and the evaporation curves

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The main sources of empirical information on the thermophysical properties of refractory metals in the vicinity of the melting and evaporation curves are experiments on isentropic and isobaric expansion. However, there are still no models that could consistently describe both types of data.
In this paper, we present the results of quantum-molecular dynamic calculations, which allowed us to describe sequentially existing data on isentropic expansion into various anvil materials of shock porous samples Mo and W and the results of experiments on fast resistive pulsed heating. Our estimates of the critical parameters for Mo and W are also presented.
We thank the program of the Presidium RAS No. 6 (of Fortov V E) for financial support.

First-principle study of the thermophysical properties of solid and liquid uranium by the quantum molecular dynamics method

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Experiments on shock compression and isentropic expansion of solid and porous samples are important for obtaining thermodynamic data in a wide range of phase diagrams, including high pressures and temperatures, but such experiments are complex and very expensive. The theoretical interpretation of experiments in condensed matter is rather difficult, since it requires knowledge of the equation of state, including taking into account the effect of a complex electronic structure on the thermophysical properties. Thus, it seems that at the present time the only available theoretical approach that can provide information of the thermophysical properties of a substance in the field of hot expanded fluid and has sufficient prognostic ability is the first-principle quantum molecular dynamics method (QMD).

The possibility of the current QMD modeling appeared due to the achievements of computational methods and supercomputers over the past two decades, and the density functional theory underlying QMD.

Thus, the purpose of this work is to study the thermodynamic properties of uranium in a wide range of temperatures and pressures using the QMD method. This paper calculates the near-zero isobar of uranium in the locality of melting, recovery the density of vibrational states for the alpha phase of uranium at $T = 645$ K and the gamma phase at $T = 1113$ K and calculates the Hugoniot of porous samples.

On the problem of equation of state for electron gas

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The equation of state for electron gas has been studying for nearly a century but still there are many questions remain. The main difficulty lays in the necessity of solving the quantum many-body problem in the conditions of strong degeneration and interaction. Not only huge computational power is required but also the notorious sign problem should be regarded. Currently only quantum Monte Carlo methods can be used for this purpose but they are very computationally demanding and contain various limitations. Therefore simplified models for uniform and non-uniform electron gas are still of great importance.

Practically a wide-range equation of state for electrons is necessary for the construction of wide-range equations of state for matter: using the adiabatic approximation one may represent free energy as a sum of ionic and electronic contributions. However there are only two theoretical models for electron gas that can be considered as wide-range: uniform electron gas and finite-temperature Thomas–Fermi model. Various corrections to the Thomas–Fermi model become unphysical at some thermodynamic conditions, the well-known Hartree–Fock–Slater model in a spherical cell has serious convergence difficulties at low densities and moderate temperatures. The so-called first-principle methods based on density functional theory can be applied only in a limited region of the phase diagram. In this work a simplified semiclassical approach taking into account the discrete energy spectrum of electrons is tested as a next candidate for the wide-range model of electronic gas.

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Theoretical investigation of thermodynamic and radiative properties of hot dense plasma using quantum-statistical methods

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Calculations of thermodynamic and radiative characteristics of hot dense plasmas, which are performed with the different quantum-statistical models, such as the Hartree–Fock–Slater [1] and the ion model of plasma [2], are presented. Calculated equations of state of different substances are used to investigate absolute and relative compression of solid Al samples in strong shock waves. Calculated Hugoniot of aluminum is in a good agreement with experimental measurements [3] and other calculated data obtained with first-principles path integral Monte-Carlo model [4]. Also we present the review of the most important applications of quantum-statistical approach to investigation of different studies for hot dense plasmas radiative properties.

This work is supported by the Presidium RAS within the fundamental research program "Condensed matter and plasma at high energy densities".

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Application of pseudoatomic molecular dynamics method for ionic transport coefficients research

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Pseudo-atomic molecular dynamics [1] is an effective technique for modeling of structural, thermophysical and transport properties of warm and hot dense matter (WDM). An effective interionic potential V has been obtained in the first approximation of the Starrett–Saumon model [2]. WDM is considered as a system of semiclassical Thomas–Fermi–Dirac electrons and classical pseudo-atoms interacting via the potential V. For the modeling of ionic trajectories the method by [3] are used.

The sets of coordinates and velocities at various moments of time are used for velocity and pressure tensor autocorrelation functions (VAF and PTAF) modeling. We also obtain ionic diffusion and share viscosity coefficients using VAF and PTAF. Ion-ion radial distribution functions and the angle rotating invariants are also calculated. These parameters are used for the structural investigations of WDM.

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The wide-range model of shell effects in hot plasma based on semiclassical approximation for bound states of electrons

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Both the Kohn–Sham–Mermin formulation and the orbital-free density functional theory are used to obtain the properties of warm dense matter with great success. Combined with molecular dynamics they provide thermodynamic properties of a mixture of electrons and nuclei in a consistent way. Thus, the development of wide-range equations of state based on such approaches is most precise, but a huge amount of computations on modern supercomputers is required. Moreover, the limitations of exchange-correlation terms in energy functional make it almost impossible to reach convergence for the low density plasma. It is found that an adequate equation of state for this region may be obtained using the simple Thomas–Fermi approach supplemented with the more realistic states of bound electrons. Using semiclassical wave functions within spherical Thomas–Fermi atom [1] the shell correction to density is obtained, which provides a proper correction to thermodynamics during thermal ionization [2] in accordance with the Saha model. The model applications within its validity region [3] are discussed.

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High-precision implementation of the Thomas–Fermi model for a mixture of atoms

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In this work, we present a TFmix code intended for numerical calculation of the thermal part of electronic thermodynamic properties of a mixture of elements by the finite-temperature Thomas–Fermi model [1]. The code is based on analytical models for both first and second derivatives of Helmholtz thermodynamic potential. All numerical calculations are made within a controlled high accuracy: tests for thermodynamic consistency give at least 11 coinciding decimal digits. The code calculates thermodynamic functions on a regular grid of isotherms and isochores; at each grid point some extensive parameters and the number of free electrons are output both for the whole mixture and for each component. Other extensive or intensive thermodynamic properties, including pressure, entropy, isochoric and isobaric heat capacities, isothermal and adiabatic sound velocities can be easily calculated from the information available at each grid point. Several unit systems are provided for convenience. A cross-platform graphical user interface is developed to simplify the use of the code. To demonstrate the possibilities of the code we have calculated shock Hugoniots for quartz and polystyrene at pressures higher than 10 Mbar. For the contribution of the ionic subsystem ideal gas and charged hard spheres have been used. We analyze the behavior of each component of a mixture along the Hugoniot.

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A multiphase equation of state for lead

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A two-phase (solid + liquid with evaporation) equation of state for lead is constructed. The equation well reproduces static and dynamic experimental data including melting. In the region of extreme states where experimental data are absent, the equation is fit to ab initio calculations. The functional dependence of free energy allows for ionization and in the limit of high temperatures corresponds to fully ionized ideal gas. The cold energy and pressure at superhigh compression provide for limiting process to the Thomas–Fermi atomic model.

Thermodinamic parametrs of mixtures with silicon nitride under shock-wave loading

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The synthesis of materials, including multicomponent materials, under intensive shock-wave impact is an effective way to create new functional and structural materials and is a promising research trend in modern material science. Thus, it seems to be important to have quite simple models that make it possible to obtain reliable estimates of the thermodynamic characteristics of a loaded multicomponent mixture, as well as used material. In [1–3] we consider the thermodynamically equilibrium model of thermodynamic equilibrium components (TEC) in its application to a series of materials. It allowed the description of the thermodynamic characteristics of a loaded medium in a wide range of pressures, including cases of mixtures with components subjected to polymorphic phase transition.
The results of numerical experiments on the modeling of the thermodynamic parameters of the shock-wave loading of silicon nitride Si_3N_4 and mixtures based on it are presented. A thermodynamically equilibrium model is used to account for the phase transition of Si_3N_4 under shock-wave loading. The thermodynamic parameters of shock-wave loading are described for pure silicon nitride, as well as for mixtures of Si_3N_4 with potassium bromide KBr, periclase MgO and aluminum nitride AlN [4]. The computation results are compared with experimental data obtained by well-known authors.

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Thermodynamic and and transportable properties of sapphire at shock compression

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Sapphire is widely used in measurements of the temperature of shock compression of metals and compounds [1–4]. In [1–4], the equation of state having Mie–Grüneisen type with parameters from work [1] is applied to determination of temperature of sapphire and its heat-conducting properties. Authors of works [1–3] confirm transparency of sapphire which is shock compressed up to the pressure of 0.3 TPa and more.

Now the shock compressibility of sapphire is experimentally defined in the range of pressure of 80–340 GPa [5] when using the two-stage gas gun and also in the range of 0.7–2 TPa [6,7] in laser shock waves. Range of pressure of 340–700 GPa is not studied experimentally.

The original explosive cumulative conical flat single impact generators were used for shock compression. As a result of the performed experiments it is shown that with a pressure up to 550 GPa the conductivity of sapphire does not exceed 60 S/cm. It gives the possibility to apply sapphire as insulating material at measurement of electric properties of many substances at shock compression.

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Measurements of temperature of water in shock waves

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In the present work, we studied the thermal radiation from water in an incident shock wave and a shock wave reflected from a barrier with higher dynamic stiffness—a transparent window of lithium fluoride. The range of the incident shock pressures was 28–36 GPa. The purpose of this work was to obtain new data for verification of the equation of state of water at lower temperatures than those on the Hugoniot at the same pressures.

In double compression to 58.6–62.7 GPa, the temperature was found in the range of 2.4–2.6 kK, and on the single-compression Hugoniot at these pressures, the temperature is 3.9–4.1 kK. Temperature values measured by the brightness and color method are well consistent with each other.

The temperature behind the front of the first and second shock waves were calculated using an equation-of-state model, in which the coefficients were selected so as to match the data on shock compression of water in one shock wave, including the results of previous temperature measurements and the data of the present work. This equation-of-state model provided an adequate description of the new experimental data on the Hugoniot of repeated shock compression in the reflected wave.

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About phase transitions in some halogenated methane at the dynamic loading

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In addition to the work [1], we present the results of measurements of the speed of sound in shock-compressed chloroform $CHCl_3$ and bromoform $CHBr_3$, performed by means of photoelectric (indicator) technique [2] at pressures up to 60 GPa. We have determined the features concerning possible leakage in specified substances of phase transformation in a shock-wave front.

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Sound velocities of shock-compressed uranium in the pressure range from 10 to 250 GPa

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We present the results of our measurements of the speed of sound in natural uranium at high strain rates, which are used to study processes in the regions of the α and γ-phases, as well as in the melting region of U in shock-wave front. The processes were recorded using the manghanin gauge (at 10–100 GPa) and the photoelectric (indicator) technique (at 90–250 GPa) [1]. In the solid phase of uranium we determined the changes of elastic moduli along its Hugoniot, such as Poisson ratio, elastic modulus, bulk modulus and shear modulus [2].

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Thermal destruction of fayalite at high hydrogen pressures

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Thermal stability of fayalite Fe_2SiO_4 under high hydrogen pressures is studied for the first time. The decomposition temperature of fayalite is shown to nonlinearly decrease from ≈ 375 °C at $P_{H2} = 1.4$–2.8 GPa to ≈ 175 °C at $P_{H2} = 7.5$ GPa. At higher temperatures, fayalite fully decomposes to a mixture of SiO_2, H_2O and metallic Fe or FeH depending on the pressure of hydrogenation.

The present work was supported by grant No. 18-02-01175 from the Russian Foundation for Basic Research and the program "Physics of fundamental interactions and nuclear technologies" of the Russian Academy of Sciences.

Temperature distribution on the surface of the laser heated diamond-like BC_x phases under high pressures into diamond anvil cell

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We use a laser heating system for investigations at high temperature and high pressure. Such system is main for static measurements of equation of state of material at high pressure and high temperature [1]. One of the main features of the system is a tunable acousto-optic filter synchronized with a video camera. This allows us to measure the temperature distribution on the surface of the studied materials [2]. A diffraction spectrometer attached to the system to provide the measurements of fluorescence and Raman scattering is used for verification of measurements of tunable acousto-optical filter. The sintering of a mixture of a powder of micro-diamonds with a powder of BC_x phase type high pressure device leads to the creation of s-BC_x phase with a low resistivity, and high elastic module [3]. We conducted the experiment with diamond-like BC_x nano-phase using tunable acousto-optical filter and diffraction spectrometer. As a result, after heating in the high-pressure cell, the sample is a solid alloy of carbon, boron and boron-doped diamond.
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Crystalline potentials and dispersion forces in the Gordon–Kim model

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The thermophysical characteristics and dispersion forces of molecular crystals were investigated, and the parameters of atom-atomic and crystalline potentials were calculated within the Gordon–Kim model [1]. For the model crystalline potential exp–6, the possibility of determining its parameters in the additive approximation of pair interaction was shown by numerical methods [2]. Analytical expressions for the dispersion forces of solidified inert gases crystals, for van der Waals constants of homo- and heteroatomic crystals, which relate them to the structural parameters of pair potentials and coordination spheres, were obtained.

It is shown that the analytical calculations of the dispersion forces are in qualitative agreement with the results of numerical simulation. The equations of state and thermophysical characteristics of solidified inert gases crystals are investigated. The results obtained are in qualitative agreement with experimental data.

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Effective pair potential for Coulomb systems and Bose–Einstein condensation

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The expression for the short-range effective interaction potential of "quasinulei" is derived based on the model of the "pure" Coulomb interaction. This model represents the equilibrium Coulomb system (CS) of interacting electrons and the identical nuclei, using the adiabatic approximation for nuclei and an arbitrary strong (in general) interaction for the electronic subsystem. On the basis of general properties of Coulomb interaction [1] it is shown that the Fourier-component of the pair effective potential between "quasinuclei" possesses discontinuity for the case of a weak electron-nuclei interaction at the wave vector $q = 0$. This discontinuity is essential for the Bose condensed systems as HeII and the rarified Alkali metals at temperatures lower than the Bose condensation transition, since there are macroscopic quantity of quasiparticles with the momentum $q = 0$ [2]. In particular, it is shown that for the single-particle excitations can exist the gap [3] which disappears in the normal state. The value of this gap is estimated. The problem of generalization of the obtained results for the case of a strong electron-nuclei (or electron-point ion system) is discussed.

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On methods for studying the ground-state energy of a non-uniform electron gas in a static external field

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The analysis of theoretical methods for the study of the ground state energy of an inhomogeneous electron gas in a static external field is carried out. It is shown that the density functional theory for an inhomogeneous electron gas, which is based on the hypothesis of the existence of an universal density functional for the potential of an external field, is not mathematically rigorous. To calculate the ground state energy of a finite inhomogeneous system with a finite number of electrons, it is necessary to determine a single-particle density matrix. When considering an inhomogeneous system of electrons satisfying the thermodynamic limit, its ground-state energy is uniquely determined by the single-particle Green function [1–6].

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Velocity autocorrelation function of a soft-sphere fluid: Kinetic approach and molecular simulation

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Velocity autocorrelation function (VAF) plays an important role in the theory of non-equilibrium processes. Recently the so-called two-phase theory (2PT) has been proposed in which VAF is used among other properties to calculate entropy. In the original theory [1] the system of hard spheres was considered as a model for a gaseous contribution to entropy. As the hard-sphere potential is quite rough to describe the properties of a real system we use the soft-sphere repulsive potential in the 2PT. In contrast to the hard-sphere potential, thermodynamic and transport properties of a soft-sphere system can not be derived analytically. Therefore classical molecular dynamics (MD) is usually applied to calculate equation of state and transport properties of a system of soft-spheres including VAF. However, the method of MD experiences significant difficulties for a rarefied system in which the particles interact very rarely, so very long computational time is required to obtain a suitable statistical error. In this work we solve a generalized kinetic equation [2] to calculate the VAF for a system of soft spheres at low and medium densities. We compare the results by kinetic approach with MD calculations on isotherms and determine densities at which both methods give similar results. The comparison shows that the kinetic approach gives reasonable results even for a dense fluid.
We thank the program of the Presidium RAS No. 6 (of Fortov V E) for financial support.

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Molecular modelling of methane–ethane mixture condensation

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Retrograde condensation is a phenomenon, that makes harder to get natural gas from well. Pressure of the natural gas falls while field development and the mixture reaches retrograde region of phase diagram. It creates an obstacle to extracting gas.
The goal of this work is finding a way to dynamically model retrograde condensation and find its kinetic borders. A mixture of methane and ethane is studied. TraPPE-UA force field is used [1]. The Nose–Hoover thermostat is used to keep temperature constant. Two types of models are considered. First, the mixture is kept at low pressure in the beginning. Then, simulation box is made smaller to create supersaturation. Second, the mixture starts at high pressure. After that, the volume is increased to make the mixture evaporate. The cluster analysis of the process is done. The dependence of the number of clusters of different sizes on time was studied. When the supersaturation is reached, the number of clusters increases. After this, the number of small clusters begins to decrease, which means that cluster growth and condensation begin.
The stability limits are calculated for 250 K. A comparison is made with theory. The phase diagram is calculated.
The present work is supported by grant from the Russian Science Foundation No. 17-79-20391.

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Structure properties of warm dense hydrogen

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The warm dense hydrogen is studied by the *ab initio* molecular dynamics simulation in the region of the fluid–fluid phase transition. A method for calculating the structure properties such as concentration and lifetime of H_2 molecules is developed. Two atoms are considered bonded if the distance between them is less than a certain r_{cut} and during the existence of this bond the distance at least once was less than $r_{\text{threshold}}$, which physically means the existence of oscillations.

As warm dense hydrogen passes the transition, the dissociation of H_2 molecules goes smoothly, while the lifetime changes abruptly by several orders. Dissociation of 5% is sufficient to increase the conductivity by several orders of magnitude. The average interatomic distance in H_2 molecule also has an abrupt jump at the transition.

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Diffusion of ions in water solution of C_2H_4 and C_2H_4O copolymers

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We study ionic conductivity of linear statistical copolymers of ethylene and ethylene oxide in water solution. The diffusion coefficients of ions K^+ and Cl^- are calculated. The statistical copolymer chain consists of 100 ethylene (C_2H_4) and ethylene oxide (C_2H_4O) units. Potential energy function for molecules in the system includes intermolecular interactions (Lennard-Jones and Coulomb potentials) and intramolecular interactions (bond stretching, angle bending and torsion of dihedral angles in the case of polymer chains). Different force fields are considered to reproduce real behavior of solution [1–5]. The initial configuration of the system is prepared via compressing gaseous mixture of water vapour and copolymer chains followed by the relaxation to equilibrium state [6]. The diffusion coefficients of system components are derived using Einstein-Smoluchowski and Green–Kubo formulas. We investigate the relation between diffusivity of K^+ and Cl^- and mole fraction of ethylene residue in the polymer chain and mass fraction of polymer in water solution. The work is supported by grant No. 18-19-00734 from the Russian Science Foundation.

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Influence of chemical composition of the surface layer on the nucleation of plasticity in CoCrFeMnNi high-entropy alloys

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Influence of element segregation in the vicinity of free surfaces with different crystallographic indices on plastic deformation nucleation in CoCrFeMnNi high-entropy alloys was studied on the base of molecular dynamics and Monte Carlo simulations. It was found that the amount of each chemical element near free surface is determined not only by the stoichiometric composition of the alloy but also by crystallographic orientation of the free surface. Changes in the chemical composition of surface layer cause an increase or decrease of elastic limit depending on free surface orientation and lead to a change in defect structure after uniaxial tension of samples. In $Co_{30}Cr_{30}Fe_{10}Mn_{10}Ni_{20}$ samples with the (001) surface plastic deformation occurs through twinning. For random distribution of elements in $Co_{10}Cr_{10}Fe_{30}Mn_{30}Ni_{20}$ samples with the (001) surface twins and hcp bands are nucleated, while after surface segregation hcp bands become the prevailing mechanism of plastic deformation.
The work was carried out with the financial support of the Russian Science Foundation (project No. 17-79-10108).

Motion of dislocations in aluminum containing the theta-prime phase: Molecular dynamics simulations and continuum modeling

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We use molecular dynamics (MD) calculations for studying of dislocation sleep in aluminum containing strengthening phases of copper in form of θ' phase. The behavior of edge and screw dislocations in aluminum with θ' precipitate is investigated. In the case of screw dislocation, we do not observe the entrance of dislocation line into the material of obstacle; the dislocation line of screw type changes its slip plane in front of obstacle and goes round it. The edge dislocation line passes through the obstacle. We find the dependencies of overcoming stress for both dislocation types on distance between and on radius of precipitations. The temperature dependence of critical stress is investigated for fixed distance and radius of θ' phase inclusion. It is shown that in the case of edge dislocation first events of overcoming of obstacle occurs due to formation of defect area in Al matrix around the θ' inclusion; the third or fourth one typically leads to shearing of obstacle. Estimating the local stresses in the inclusion upon interaction with the edge dislocation, we find that its value reaches 2.4 GPa. We offer a simple mechanical model of overcoming obstacles by dislocation with only one selected parameter, which is the dislocation energy per unit length. The equations are formulated in assumption of constant properties of θ' phase during interactions with dislocation. It is necessary to include the temperature dependence of the dislocation energy in order to obtain agreement between the simulated data and the MD calculations.
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Effect of copper nanoinclusions on tensile strength of aluminum matrix at ultra-high strain rates

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We use molecular dynamics to study the effect of Cu nanoinclusions on the shear strength of an aluminum matrix. In the case of copper nanoinclusions in aluminum matrix, lower threshold shear stresses in comparison with the pure aluminum at the incipience of plasticity and higher shear stress level at the final stage of deformation with developed dislocation structure are observed. Also, the presence of copper nanoinclusions reduces the energy barrier for the nucleation of dislocations due to concentration of stresses in vicinity of inclusion.

Using the results of molecular dynamics simulations, we develop a continuum model, which takes into account the nucleation, annihilation, and multiplication of dislocations. In the case of copper nanoinclusion in aluminum matrix, the continuum model considers the additional nucleation of dislocations in the region of the stress concentrators in vicinity of the inclusion. Variation of the stress concentration coefficient allows us to obtain the correspondence of the model results with the results of molecular dynamics simulations for maximum stresses and the initial stage of stress relaxation.

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Dislocation movement in aluminum: Molecular-dynamics simulation and modeling with accounting of local stress

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We present an approach combining molecular-dynamics (MD) simulations and continuum modeling of dislocation motion in pure aluminum. The problem was investigated previously [1, 2] in terms of average stress in MD system. Recently [3], it was shown that motion of dislocation occurs under the action of local stress acting around it. The present study is carried out using the solution of the equations of dislocation motion in approximation of local stress in comparison with MD results. MD calculations are performed for pure aluminum in statement with motion of top and bottom layers with constant velocities. An increase in strain rate leads to increased stresses. In the result, starting from some value of shear rate, we cannot make the time averaging for stress. The increase is the consequence of insufficient plastic relaxation rate due to fixed number of dislocations in the system and dislocation velocity limited by transverse sound velocity. There are fluctuations in graphics with histories of stresses. This fact can be explain by dislocation entrance in the trace of previous dislocation, that occurs due to the presence of periodical boundary conditions. Thus, the model parameters are modified in comparison with [3] to better match the results of continuum modeling and the results of MD modeling. This work is supported by the Russian Science Foundation No. 18-71-10038.

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Comparison of the Zerilli–Armstrong model and the Maxwell relaxation model with variable relaxation time for description of elastic precursor of shock waves in aluminum

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In this report, shock-wave profile in aluminum is modeled by using both Maxwell relaxation model [1] and the Zerilli–Armstrong model [2]. In the first case, change of both the relaxation time and the yield strength is taken into account. In the second case, the von Mises yield criterion with variable yield stress is considered. Event of the impact of a flying Al plate upon a target Al plate is studied. Calculations are made at different thicknesses of the striker and the target, as well as at different speeds of the flying plate. The temporal evolution of the velocity of the rear surface of the target is compared with the experimental data [3]. The comparison shows that the Zerilli–Armstrong model is not applicable for describing the elastic precursor of the shock wave, and the Maxwell relaxation model with a variable relaxation time gives much better agreement with the experimental data, as was shown earlier in [1].

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Interaction of the edge dislocation with copper atoms in the aluminum crystal

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In the present work, the interaction of the moving edge dislocation with an obstacle is investigated using the molecular dynamics simulations [1]. The samples are aluminum monocrystals with a volume of $52 \times 60 \times 15$ nm^3 and axes of system are oriented along directions $[\bar{1}10]$, $[111]$, $[11\bar{2}]$. The structure of Cu solid solution is reproduced with following procedure: aluminum atoms are randomly selected and replaced by copper atoms (obstacles). The edge dislocation is created in the center of the crystal [2]. The concentration of copper atoms varied: 0.25, 0.5 and 1%. Atomic interactions are described by the ADP potential for aluminum and copper [3]. The dislocation movement occurs under action of shear deformation. The areas of the top and bottom of the crystal of 3 nm thickness are selected and moved with a constant velocity (3 and 0 m/s). It is found that zones with a low concentration of Cu atoms only slow down dislocation in an Al matrix and the zones with a high concentration of copper atoms not only produces stronger resistance to dislocation movement, but also they cause to change the slip plane of the dislocation segment. When a significant part of dislocation line moves to neighboring slip plane that can stimulate the full transition of dislocation to this slip plane. It is also noted that such transitions of the dislocation segments from one slip plane to another are accompanied by the formation of vacancies. Also the maximum value of the shear stress σ_{xy} is estimated; its value is ≈ 250 MPa.

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Phase transformation crystallization–amorphization in metallic materials induced by severe plastic deformation

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The structural and thermodynamic aspects of the process of strain-induced amorphization occurring upon severe plastic deformation is widely studied in recent years and are the matter of considerable debate. Basically, this process is developed in amorphizable multi-component Pd–Cu, Ti–Zr, Zr–Cu, Mg–Cu, Ti–Ni, and Fe–B based metallic systems. Since the end of the last century, the strain-induced amorphization was intensely studied upon high-pressure torsion (HPT). The Ti–Ni based alloys were investigated most actively. In this work, the evolution of the structure and mechanical behavior upon deformation has been studied experimentally in situ by room-temperature HPT of the initially crystalline Ti2NiCu alloy. An abrupt increase in the shear stress upon HPT has been revealed. It was found that the observed effect is due to the strain-induced "crystalline amorphous state" phase transformation and the corresponding change in the mechanism of severe plastic deformation. It is shown that the amorphization of the material begins at the boundaries of grains and fragments of the crystalline phase as a result of grain boundary sliding processes. It was established that the amorphous boundaries form a "grain-boundary framework", which upon deformation is expanded and transformed into bulk amorphous phase.

Impact of composition variation and high pressure up to 10 GPa on thermoelectric properties of ferrum–vanadium–aluminium alloys

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Recent works confirm existence of a sharply varying electron density of states and a strong scattering of charge carriers by magnetic inhomogeneities in Fe_2VAl alloy with a composition variation near the stoichiometric one [1]. Non-stoichiometric Fe_2VAl samples were found to show significant improvements in the Seebeck coefficient [2]. In the present work, the behavior of Seebeck coefficient (S) and electrical conductivity of set of $Fe_{2-x}V_{1+x}Al$ samples ($-0.1 \leqslant x \leqslant 0.2$) were investigated under quasi-hydrostatic pressure (P) up to 10 GPa. The high pressure study was carried out at room temperature using the automatic installation of a miniature high pressure cell anvil with hard-alloy anvils [3]. Experimental data revealed that composition variation caused strong qualitatively changes in $S(P)$ curve. It was found that application of moderate pressure up to 1–2 GPa caused two-fold increasing of thermoelectric power factor value for $Fe_{2.1}V_{0.9}Al$ compound.

The research was carried out within the state assignment of the Minobrnauki of the Russian Federation (theme "Electron" No. AAAA-A18-118020190098-5), supported in part by the Russian Foundation for Basic Research (project No. 18-32-00618).

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High density hydrogen storage of Ti-based alloys under high pressure

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TiZrNi alloys exhibit periodic, quasi-periodic and glassy structures depends TiZrNi alloys exhibit periodic, quasi-periodic and glassy structures depends on their cooling rates. The semi-rapid quenched alloys form quasicrystals and the formation and stability of quasi-periodic materials have been refocused after the awarding of Nobel Prize of Chemistry in 2011 to Dr Shechtman for the discovery of quasicrystals. Ti–Zr-based quasicrystals are the second largest family forming stable quasicrystal followed by Al-based ones. One of the most interesting structural properties of Ti/Zr-based quasicrystals is that they absorb a large amount of hydrogen exceeding the density of liquid hydrogen. In fact, $Ti_{53}Zr_{27}Ni_{20}$ quasicrystals are known to absorb near 2.0 wt % hydrogen, reversibly. Further, theoretical calculation and modeling of their approximant phases predict that a significant amount of interstitial sites are still available for hosting hydrogen suggesting the materials have technical advantages for hydrogen storage application. To realize the prediction, we pressurized TiZrNi alloys including C14 Laves phase and quasicrystals using a diamond anvil cell up to 48 GPa under hydrogen environment and estimated the hydrogen loading capacity and transport properties. By analyzing the peak shifts in synchrotron-based x-ray diffraction data revealed that quasicrystal phase sustained to the applied pressure with uniform shift of the main peaks suggesting that hydrogen atoms diffuse into the interstitial sites homogeneously without phase transformation. The maximum value of hydrogen loading at 48 GPa was near 4 wt % with a completely reversible process. Mechanism of hydrogen loading, effects of hydrogen on structural stability and transport properties as a function of pressure will be presented.

High-pressure influence on thermo-emf of multi-component polycrystalline materials Cu–Ge–As–Se system

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This work is devoted to the high pressure (up to 50 GPa) influence on the thermo-emf (α) of the polycrystalline $(GeSe)_x(CuAsSe_2)_{1-x}$, $x = 0.3$, 0.5 and 0.6. These materials are well known semiconductors with interesting thermal and baric dependences of electric properties [1,2]. It has previously been shown that these materials have a high value of thermo-emf at atmospheric pressure in the temperature range 300–400 K [3]. High pressures have been achieved using the high-pressure cell described in detail in paper [4].
The behavior of the magnetoresistance and thermo-emf in the pressure range up to 50 GPa has been analyzed. It was found that the absolute value of the thermo-emf of all materials decreases with pressure increasing from 4 to 50 GPa (for $x = 0.3$ from 250 to 25 μV/K, $x = 0.5$ from 120 to 20 μV/K, $x = 0.6$ from 340 to 90 μV/K), the sign corresponds to the electronic type of conductivity. As well, the phenomenon of negative magnetoresistance is observed for this material. A correlation between the baric behavior of magnetoresistance and thermo-emf has been established for all materials.

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Microstructure and properties of stable amorphous films of the Ag–Sn–Sb–S system

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The problem of creating renewable energy sources sets task which related with searching of new materials for thermoelectric and photoelectric devices. Recently multicomponent chalcogenides became the most promising researching objects [1–4]. In this paper, we have synthesized thin films (10–20 and 50 nm) of bulk crystalline material $AgSnSbS_3$ by vacuum deposition on a mica with carbon sublayer. Studies of the microstructure and optical parameters were carried out with a transmission electron microscope (JEM-2100) and a spectrophotometer (Agilent Cary 5000). Films are homogeneous amorphous by the study. Amorphous state of obtained materials are stable under heating up to 380 K and irradiation by focused and scanning electron beam.

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Baric phase transitions in three-dimensional topological semimetal Cd_3As_2 doped with MnAs

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For the purpose of identifying phase transitions in three-dimensional topological semimetal Cd_3As_2 heavily doped with Mn the pressure dependences (up to 50 GPa) of thermo-emf, electrical resistance and magnetoresistance at ambient temperature and magnetic susceptibility within the temperature range of 5–350 K at the ambient pressure in the $Cd_3As_2 + n$MnAs composite (where $n = 30$ and 44.7 mol %) are studied. Synthesis and materials attestation methods are described in [1]. The ferromagnetic to paramagnetic transitions in the composites were determined at 310 K. The first baric phase transition at 4.4 GPa was found by examining the pressure dependence of the electrical resistivity and magnetoresistance earlier [2, 3]. The second baric phase transition in the pressure range from 30 to 33 GPa is transformation in the electronic subsystem, and it is characterized by the features of behavior of all studied characteristics.

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Effect of high pressure on the Seebeck coefficient of single-walled and double-walled carbon nanotubes

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The effect high pressure on the baric dependences of Seebeck coefficient S of the single-walled and double-walled carbon nanotubes was studied for the purpose of identifying baric phase transitions in the 4–46 GPa interval. Pressure about 50 GPa has been generated in a high-pressure chamber with conductive synthetic diamonds. The objects of research were single-walled and double-walled carbon-nanotubes. Considering the design features and the connection diagram, the sign of the Seebeck coefficient and its magnitude correspond to carriers of the electron type. The nature of the baric dependence of coefficient S indicates a partial reversibility of the transformations occurring in the sample. Also in these dependences one can observe a number of certain features associated with changes occurring in the structure of the sample at high pressure.

State of trapped matter inside graphene nanobubbles

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Graphene nanobubbles form when a substance is trapped between a graphene sheet (two-dimensional crystal) and an atomically flat substrate. The physical state of the substance inside graphene nanobubbles can vary from the gas phase to crystal clusters. In this paper, we present a theoretical description of the gas-liquid phase transition of argon inside graphene nanobubbles. The energy minimization concept is used to calculate the equilibrium properties of the bubble at constant temperature for a given mass of captured substance. We consider the total energy as a sum of the elastic energy of the graphene sheet, the bulk energy of the inner substance and the energy of adhesion between this substance, the substrate and graphene. The developed model allows us to reveal a correlation between the size of the bubble and the physical state of the substance inside it. A special case of a graphene nanobubble that consists of argon trapped between a graphene sheet and a graphite substrate is considered. We predict the "forbidden range" of radii, within which no stable graphene nanobubbles exist, that separates bubble sizes with liquid argon inside from bubble sizes with gaseous argon. The height-to-radius ratio of the bubble is found to be constant for radii greater than 200 nm, which is consistent with experimental observations. The proposed model can be extended to various types of trapped substances and two-dimensional crystals.

Interaction of matter with graphene

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Specific adhesion energy is important characteristic of interaction of matter with the substrate. Particularly it is crucial part in developing theoretical model for graphene nanobubbles [1]. Adsorption is a basic phenomenon underlying this interaction.
In the present work, we use molecular dynamics simulations to calculate specific adhesion energy for ethane; the temperature and density dependency is investigated. The Langmuir adsorption model is applied to interpret results. Also appearance of multilayer adsorption is detected for high densities. Developed model and numerical approach to calculate adhesion energy and surface coverage can be applied for different types of matter and substrate.

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Interaction of graphene sheet with metal droplets and substrates

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Molecular-dynamic (MD) simulations revealed that there is a build-up of transverse vibrations of graphene atoms with their transition to bending vibrations of membrane type. The amplitudes of such oscillations can reach large values, which considerably exceed the interatomic distances already for samples of micron sizes and amount to 10^{-2} from the length of the sample [1]. Such oscillations can be excited by the action of the tip of a cantilever needle on a free sheet of graphene [1]. The dynamics of a graphene sheet in contact with a liquid metal drop was considered by MD methods using the potentials of LCBOP and MEAM. Found wetting angles and surface tension of the graphene–liquid metal interfaces. The behavior of multilayer graphene when approaching the (100) plane of iron is considered. It is shown that the effect of the tear off of a single or several graphene layers with their adhesion to the surface of iron takes place for the sufficient sizes of iron. For graphene sheet partially lying on the edge of an aluminum substrate the effect of the sheet rolling over aluminum was observed. Ultimately, the graphene sheet is completely located on the surface of aluminum, which corresponds to a minimum of adhesive interaction. This effect can be used to obtain graphene coatings.

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Preparation of high density samples of ZrC_x and TaC_x

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Ceramics made of carbides of zirconium and tantalum are refractory and have a number of valuable properties. High melting temperature [1, 2] makes them useful for various applications implying extreme conditions. On the other hand, this feature makes it difficult to process the substances and to obtain the material with a necessary composition and density. Moreover, some application, for instance, in additive technologies requires samples with a homogeneously distributed composition. The method proposed in the work is similar to one presented in [3] for preparation of samples from zirconium carbide with several improvements. Powders of metal (Zr or Ta) and carbon black were mixed in the required ratio to obtain carbides with a definite C/Me ratio. The mixture was pressed and sintered at temperatures up to 2500 K. The sintered samples had a density about 85% of the theoretical one. Also the surface of sintered samples was partially melted to obtain substance with a high density. The analysis of the samples has shown that the ratio of C/Me in carbide did not change during melting and carbon and metal are uniformly distributed across the melted area.

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Thermal deformation and polymorphic transitions of 1,1-diamino-2,2-dinitroethylene in the temperature range from 145 to 475 K

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Under atmospheric pressure, polymorphic transitions α–β, β–γ, inverse γ–α and some points of phase equilibrium for 1,1-diamino-2,2-dinitroethylene (DADNE, FOX-7) were studied in the temperature range from 145 to 475 K. Anisotropic characteristics of thermal deformation of DADNE crystals are determined by powder thermoradiography. The points of structural changes was by increments of 20, 10 and 2 K. Calculations of x-ray diffraction data were performed using full-profile analysis integrated into the algorithm by loop quantum modeling of molecular structures [1]. As reference methods used a full-profile analysis method Pawley [2], Le Bail [3], Rietveld [4] (WPPD) and WPPM [5]. The main crystallographic axis and the characteristic surface of the tensor of thermal expansion were determined. The tensor of thermal expansion and the temperature dependence are presented numerically, algebraically and graphically. The obtained results can be used to construct equations of state of condensed DADNE.

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Anisotropic thermal deformation α, β and δ-cyclotetramethylene tetranitramine crystals at atmospheric pressure

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Anisotropic thermal deformation of α, β and δ-cyclotetramethylene tetranitramine (HMX) in the range from 150 to 520 K was studied by powder x-ray diffraction. The points of structural changes of energetic materials was by increments of 10 K. Calculations of x-ray diffraction data were performed using full-profile analysis integrated into the algorithm by loop quantum modeling of molecular structures [1]. As reference methods used a full-profile analysis method Pawley [2], Le Bail [3], Rietveld [4] (WPPD) and WPPM [5]. The main crystallographic axis and the characteristic surface of the tensor of thermal expansion were determined. The tensor of thermal expansion and the temperature dependence are presented numerically, algebraically and graphically. The obtained results can be used to construct equations of state of condensed α, β and δ-HMX.

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Experimental study of thermophysical properties of W–Re alloy near its melting point

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In this work, we used the experimental technique for investigation of thermophysical properties of refractory materials in the high-temperature region up to the melting point at high pressures. Using this method, an experimental determination of the thermal expansion coefficient, electrical resistivity and emission spectra at premelting region of W–Re alloy have been carried out. Such data are necessary for its use in high-temperature engineering, as well as for the construction of wide-range equations of state of this material. This work presents data on the measurement of the thermal expansion coefficient of the W–Re (27 atomic percent of Re) alloy in the temperature range of 2400–3100 K in the premelting region. In addition, the emission spectra of the alloy in this temperature range were measured. Comparison of the experimental data on the relative thermal expansion of this W–Re alloy with the literature data for the alloy with similar stoichiometry confirms the reliability of the data obtained.

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Investigation of thermophysical properties of refractory metal carbides near its melting point with pulse heating technique

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Modern technologies require knowledge of the thermophysical properties of refractory materials, in particular carbides (e.g., TaC, TiC, HfC), at high temperatures and in the melting region. The experimental study of the thermophysical properties of refractory carbides, and the effect of stoichiometry of carbides on such properties as enthalpy, electrical conductivity and thermal expansion under fast electric heating are of great interest nowadays. The dependence of these properties of refractory carbides on their stoichiometry is an important factor for their practical use and theoretical study.
The novelty of the proposed approach is the use of precision technology of spectral optical pyrometry, high-speed digital visualization of the thermal expansion of the materials under study, as well as the possibility of using various heating rates 10^5–10^7 K/s [1]. The chosen approach allows us to investigate the thermophysical properties of refractory carbides over a wide range of high temperatures for stoichiometries previously unstudied.

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Determination of the melting point of substances by the optical method

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The laser heating system for high temperature and high pressure studies with double acoustooptical filter was used to determine the distribution of laser radiation and temperature distribution on surface the sample during laser heating [1]. The system is main for measurements of the equation of state of material under high pressure and high temperature [2]. A combination of laser heating with a double acousto-optic spectrometer was demonstrated that allows measuring the temperature distribution on the sample surface in the region of the laser spot. A method of searching for the melting point was demonstrated.

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Comparison of methods for obtaining temperature and emissivity when a tungsten lamp is heated

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A comparison of methods for obtaining temperature distributions and searching for the emissivity of heated samples is presented. The method of data acquisition is based on a unique measurement setup developed at the STC UI RAS. This method allows the use of both laser and electric heating methods in combination with an acousto-optic system [1], which allows to obtain measurements at more than 100 wavelengths, which significantly increases the reliability of the results. This installation allows obtaining high temperatures. A mathematical analysis of the reliability of the results using one- and two-dimensional minimization methods was performed. The analysis of the dependences of the emissivity errors on temperature for the Planck and Wine methods was performed.

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Investigation of the electrical and magnetic properties of metal chalcogenides and their compounds intercalated by laser pulses

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The composition of the samples of gallium selenide GaSe and pyrite FeS_2 was identified by x-ray fluorescence analysis. The concentration and mobility of charge carriers in a sample of gallium selenide GaSe and pyrite FeS_2 were determined using the Hall electromotive force measurement method. A study was made of the magnetic properties of the samples of gallium selenide GaSe and pyrite FeS_2 using electron paramagnetic resonance spectrometry. The search for ferromagnetic resonance was carried out in the microwave range of 9–9.8 GHz in a smoothly controlled magnetic field from 4 to 12 kOe. Nickel deposition on the surface of a flat-shaped pyrite sample was carried out by the method of magnetron sputtering. The thickness of the nickel layer was 1 μm.

Galvanomagnetic properties of Fe–V–Al based alloys with variations in composition near the stoichiometry

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Ternary iron–vanadium–aluminum alloys were studied. It was found that it was a strong effect of aluminum content on the magnitude and character of the development of spontaneous magnetization. Investigation and analyzes the magnetoresistance and anomalous Hall effect of Fe–V–Al alloys with a composition change near the stoichiometric, both for iron atoms and aluminum atoms, was performed in this work. From the temperature dependence of the resistivity, we observed characteristic maxima, which indicate the presence of a ferromagnetic phase transition, from which it was concluded that even a slight deviation from stoichiometry in the direction of increasing Al content leads to a significant increase in the Curie temperature [1,2]. A sample rich in V exhibits a semiconductor temperature dependence. An investigation of the Hall effect showed that the additional doping of the alloy with Al atoms leads to a change in the sign of the anomalous contribution from the negative (Al-enriched sample) to the positive (the sample enriched with Fe and Al) above 10 K. The obtained data confirm the existence of a sharply varying electron density of states and a strong scattering of charge carriers by magnetic inhomogeneities in alloys with a composition variation near the stoichiometric one.

This research was carried out within the state assignment of the Minobrnauki of the Russian Federation (theme "Electron" AAAA-A18-118020190098-5) and supported in part by the Russian Foundation for Basic Research (project No. 18-32-00618).

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Pressure and temperature effects on the elastic properties of the adamantane

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Adamantane $C_{10}H_{16}$ is one of the archetypal diamondoids. Under normal conditions, it crystallizes in a face-centered cubic structure containing orientationally disordered adamantane molecules. This structure transforms into an ordered body-centered tetragonal phase either upon cooling to 208 K or pressurizing to above 0.5 GPa [1, 2]. We report the systematic study of the effect of pressure and temperature on elastic properties of adamantane by ultrasonic method. The measurements of sound velocities and relative volume were carried out on the high-pressure piston-cylinder setup in the P range 0–1.5 GPa and T of 77–293 K. The measurements were performed by the pulsed ultrasonic method using $LiNbO_3$ plates as piezoelectric sensors with carrier frequencies of 5–10 MHz [3]. In our investigations, the elastic moduli were determined under pressure and during a phase transition. The pressure derivative of the bulk modulus was equal 11 for the first and second phases. It is interesting to note that we did not observe a jump in the dependence of the bulk modulus during the phase transition from a fcc structure to an ordered body-centered tetragonal phase, but an increase of the shear modulus by 30% during the transition was determined. At low temperatures ($T = 77$ K), the pressure derivative of the bulk modulus decreases from 11 to 6 upon increasing pressure while the shear modulus increases linearly.

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Crystal nucleation and the temperature dependencies of the rate characteristics of crystallization

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The kinetics of the crystallization of a supercooled liquid is characterized by such the characteristics as the growth rate, the waiting time (lag-time) of nucleation, the attachment rate, the growth rate and the rate of crystallization (the last quantity is usually determined per unit volume of the system). The temperature dependencies of each of these quantities for different systems can vary significantly. Depending on the concrete system specifics, the difference can be several orders of magnitude. Nevertheless, there are common physical principles that indicate on the possibility of a unified description of the temperature dependencies of these rate characteristics. This report will present some existed approaches.

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The extraction of hadronic matter viscosity from nuclei levels data, relativistic heavy-ion collisions and neutron stars dynamics

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A fluid drop model of capillary oscillations of the core with viscosity was developed in our previous work [1]. A comparison of the frequencies of the quadrupole and octupole vibrations of even spherical nuclei leads to the fact that the viscosity of the substance of the nucleus η falls in the interval 4.2–7.6 MeV fm$^{-2}\,c^{-1}$. These results we applied to neutron stars gravitational quadrupole oscilations that take place right after their formation in collapse processes. Attenuation decrement for neutron star with mass M can be expressed in the form

$$\gamma = \frac{1}{3}\frac{\hbar c^3}{E_p^2}\frac{\eta a}{r_g}, \tag{1}$$

were $r_g = 2GM/c^2$, $E_p = 1.22 \times 10^{19}$ GeV, $\eta = 4.5$ MeV fm$^{-2}\,c^{-1}$. For neutron core mass equal solar mass one can find that $\gamma = 6.8 \times 10^{-17} s^{-1}$ and corresponding attenuation is equal to $\tau = 4.8 \times 10^8$ years. Comparison of these results with RHIC data gives the following expression quark-gluon plasma viscosity

$$\eta = AT, \tag{2}$$

where $A = 1.5\,10^{-2}$ MeV fm$^{-2}\,c^{-1}$, T is the temperature of quark–gluon plasma in MeV.

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Experimental setup for determining the surface tension of highly curved interfaces by static and dynamic methods

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The study of wetting of semiconductor, carbon and ceramic materials with microdrops of low-melting metals and alloys is important for understanding the mechanism of interaction between metal and substrate atoms at the interface [1]. The purpose of this work is to create an experimental setup and an appropriate methodology for determining the surface and interfacial tensions of microdroplets of low-melting metals and alloys immersed in a gas or liquid medium. Methods are proposed for determining the surface tension of microdroplets Ga, In, Sn that are both in a free (suspended) state and on a solid substrate or nozzle end. Plates of pyrite (FeS_2), silicon, sapphire and graphite are used as substrates. The surface tension of the interface is calculated on the basis of the solution of the problem of statics and the capillary dynamics of the metal microdroplet—substrate system. Experimental data are compared with the results of molecular dynamic simulation using the LAMMPS program.

Work is supported by the Russian Foundation for Basic Research, grant No. 18-02-01042.

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The equation of state of a mixture of dense gases taking into account the detailed chemical composition

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Developed numerical methods for calculating gas-dynamic flows and wide-range universal equations of state allow one to solve a wide range of scientific and technological problems. The construction of quantitative models of dense reacting gases is an urgent task, which at the present level of scientific understanding and technical capabilities can be solved at a high level.
In this paper, the statistical Monte-Carlo method was used to construct the equation of state for dense reacting gases. The substance was considered as a set of point objects (molecules) interacting with the central pair potential. Additionally, molecules have internal degrees of freedom, whose energy depends only on temperature. To determine the equilibrium chemical composition, pressure, and total energy of the system, the mechanics of motion of a small ensemble of particles (100 pieces) was modeled. For homogeneous systems, it is quite enough to determine the equilibrium chemical composition. The paper pays attention to the selection of parameters of pair interaction potentials for describing the behavior of dense gases under conditions of shock waves and detonation of condensed explosives. To calculate the parameters of compositions based on compounds from C, N, O, H, a thermodynamic parameters calculator with access via the Internet (http://ancient.hydro.nsc.ru/chem) was developed.

The equation of state—which? Selection methods in the model of interacting centers

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Three components of the problem of the equations of state (EOS): obtaining new ones, improving the known ones and choosing the optimal ones among them are still relevant. This work presents new results obtained for the EOS based on the molecular model of interacting point centres (IPC). At a new stage, the calculated capabilities of the IPC model are being implemented. The method of choice in the one-parameter family of EOS IPC of an optimal equation for concrete substance is proposed. A consistent set of 4 parameters is found using the experimental value of the critical compressibility factor. The method of choosing the EOS was tested by calculating the critical isotherms of a number of substances, including argon, nitrogen, ammonia, carbon dioxide, perfluorocyclobutane, trifluoromethane. Present value analysis in the interval of reduced densities from 0.01 to 3/2 showed that the selected EOS IPC turned out to be better (or not worse) than the most well-known—the Redlich–Kwong, Peng–Robinson, and Martin's EOSs, obtained by the volume translation. Comparison of two configurational contributions of EOS, in which the forces of attraction and repulsion are manifested, led to the introduction of a new parameter, one value of which (at the critical point) is sufficiently for a preliminary prediction of whether these EOSs are analogs. The first 4 studied for argon EOS give such clearly different ranges of values for the new parameter: 7–3.7–1.9 and 7.25–3.37–1.88 for one pair of equations and 5.1–2.8–1.34 and 4.89–2.67–1.56 for another pair. At the same time, the found intervals of values coincide with the forecast based on molecular information.

A fundamental equation of state developed on the basis of scale hypothesis and similarity theory

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A method for constructing the fundamental equation of state (FEoS) is considered, based on the representation of a large-scale hypothesis in the form of an expression connecting the singular component of entropy ΔS with a certain function X:

$$\Delta S X^{(1-\alpha)/\chi} = \varphi_0 + \varphi_1 m^2, \qquad m = \Delta\rho X^{\alpha/\beta}, \tag{1}$$

where $\Delta\rho = \omega - 1$; $\omega = \rho/\rho_c$; α, β, χ and Δ are critical indices; X is the thermodynamic function, which has a feature at a critical point, which is characterized by a critical index χ.

Based on (1), the FEoS was developed in the form of an expression for the Helmholtz free energy $F(\rho, T)$:

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

where $a(x)$ is the scale function of free energy; ϕ is the crossover function.

Based on the Scofield linear model and the similarity theory [1], all parameters of the scale function $a(x)$ are calculated. The proposed method for constructing FEoS (2) was tested on the example of describing the thermodynamic surface of argon and R236ea. The tables of equilibrium properties of argon are calculated in the region of state parameters: $\phi = \phi(\omega, T)$ by temperature from 83 to 17000 K. Detailed thermodynamic tables of R236ea $\phi = \phi(\omega)$ are also calculated. It is shown that, according to the accuracy of the calculation of the equilibrium properties in the regular part of the thermodynamic surface, the proposed FEoS is not inferior to the known National Institute of Standards and Technology FEoS, and in the critical area to the scale equations of state.

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Fundamental equation of state developed on the basis of Migdal's phenomenological theory

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We discuss the possibility of using Migdals phenomenological critical point theory [1] to construct the fundamental equation of state (FEoS) satisfying scale theory. In the framework of the approach proposed in [2], on the basis of Migdal's phenomenological theory and the Benedek's hypothesis, a scale function of chemical potential $h(x)$ was developed in the form of the expression:

$$h(x) = A[(x + x_1)^{\gamma} - \varphi_0(x + x_1)^{\gamma - 4\beta}], \tag{1}$$

where $x = \tau/|\Delta\rho|^{1/\beta}$; $\tau = T/T_c - 1$; $\Delta\rho = \rho/\rho_c - 1$; ρ_c and T_c are critical parameters; β and γ are critical indices; A, φ_0 and x_1 are constant parameters.

On the basis of the new representation of the scale hypothesis and the scale function $h(x)$ (1), we developed the FEoS, which was tested on the example of describing the equilibrium properties of SF_6. We compared the obtained results with the results of calculations of the equilibrium properties of SF_6 using the National Institute of Standards and Technology (NIST) viral type equations of state and the BMM FEoS (Bezverkhy *et al* 2017), which takes into account the features of the critical point. We showed that when describing the vicinity of the critical point, the uncertainty of calculations of the equilibrium properties of the proposed FEoS is significantly less than in the NIST EoS. When describing the equilibrium properties of SF_6 in the regular part of the thermodynamic surface, the proposed FEoS with less uncertainty describes the equilibrium properties of SF_6 than the BMM FEoS.

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Comparative analysis of various models of the phase equilibrium line

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In the present paper, we discuss so-called Yang–Yang anomaly that concerns such functions as $\mathrm{d}^2 p_s/\mathrm{d}T^2$ and $\mathrm{d}^2\mu^{\pm}/\mathrm{d}T^2$. Here p_s is the pressure on the elastic line, $\mu^{\pm}$ is the chemical potential values, respectively, on the liquid or vapor branches of the coexistence curve. These functions should determine the divergence of the third function, isochoric heat capacity, in the form $C_V(T_s) \sim \tau^{-\alpha}$ on the saturation line $T = T_s$ in the critical region, here $\tau = 1 - T/T_c$ is the relative temperature, T_c is the critical temperature, α is the critical index. The question of the form of coordination $C_V(T_s) \sim \tau^{-\alpha}$ with the specified functions is open. The consequence of the Yang–Yang anomaly is the scaling dependence of the average diameter f_d in the form $f_d = (\Delta\rho^- + \Delta\rho^+)/2 \sim \tau^{2\beta}$, here $\Delta\rho^{\mp} = (\rho^{\mp}\ \rho_c)/\rho_c$ is the relative density of the liquid (+) and gas (−), β is the critical index. On the basis of the Gibbs–Duhem equation, the scale hypothesis and the Clapeyron–Clausius equation, the authors analyze models f_d in the form of scaling functions ($f_d \sim \tau^{2\beta}$, $f_d \sim \tau^{1-\alpha}$). Testing of these models was carried out on the example of a joint description of experimental data on ρ^-, ρ^+ and p_s that relate to R236ea, C_6F_6 and R1234yf. As a result, we have developed a system of mutually agreed equations describing the phase equilibrium line of pure substances from the triple point to the critical point. Additionally, an analysis of the behavior f_d in the vicinity of the critical point was carried out on the basis of local equations of the saturation line [1]. The analysis of the obtained results is given.

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Investigation of the gas density, the liquid density and the gravitational effect in the critical region of C_6H_6

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It is analyzed some literary sources, which contain data on the liquid density (ρ_l) and the gas density (ρ_g) on the saturation line of C_6F_6. We have considered also a work of Stankus et al (2006) that includes experimental ρ_l, ρ_g, T data as well as some models to represent these points. There are also height dependences of the density, $\rho_l(h)$, $\rho_g(h)$, investigated for two-phase sample, here h is the distance of the gamma-ray beam from the bottom of the cell, where the sample is placed. The numerical data on the gravitational effect are got with the help of the gamma ray attenuation technique.
The dependences have shown that the gravitational effect is remarkable along isotherms in the critical region. Functions, $\rho_l(h)$, $\rho_g(h)$, let us conclude: a continuous transition takes place at condition 1 in the cell. We have studied a behavior of two-phase sample at condition 2. In the case: (i) we have reduced the gravitational effect in the cell and (ii) we have investigated h_M position of the two-phase interface or the meniscus location, h_M, here h_M is the distance of the meniscus from the bottom of the cell. Numerical h_M, T data let us correct experimental ρ_l, ρ_g, T data in the critical region. On the base of these ρ_l, ρ_g, T data, it is build some scaling models [1], which have approximated the experimental values in the temperature interval from 299 to 516.65 K (the critical temperature). The analysis of the obtained results is done.

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Simulation of filtration process of hydrocarbon fluid with retrograde properties

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A mathematical model for a one-dimensional filtration process of a binary hydrocarbon system having retrograde properties in a certain range of pressures and temperatures was developed. Experimental studies of the filtration process of the model mixture of methane and n-butane were carried out in order to verify the developed mathematical model and various regimes of movement of the model mixture in a porous medium were obtained.

Effect of overpressure in dual porous media on well productivity

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Overpressure takes place in ultra low permeable rocks (for example oil shale). Overpressure can contribute to well productivity not only due to additional pressure drop but also due to the appearance of secondary cracks. This phenomenon, called natural hydraulic fracturing, is well known and is described in the literature [1]. The concept of dual porosity is a common way for simulation of oil and gas shale production [2]. The porous fractured media is considered as superposition of two permeable continua with mass exchange. The first media is ultra low permeable matrix. The second is highly permeable continuum that is used for simulate a system of main cracks. In this work damage mechanics [3] is applied for simulation of natural hydraulic fracturing in low permeability matrix. The process of the secondary micro cracks development influences on the matrix permeability and enhances mass exchange between the continua. Numerical simulation of fluids motion near long well in dual porous media with overpressure was performed. It was shown that well pressure drop could lead to damage zone creation. This zone is localized near the well but improving productivity has a lasting effect because of increasing of effective radius of the well.

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Influence of pressure relaxation time on the filtration process of mixtures with features on the phase diagram

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In the collaborative filtering, multiple miscible fluids may cause non-equilibrium filtering mode. In the developed gas-dynamic filtration models it is necessary to take into account the total relaxation time, which affects the calculation of filtration processes. This account is possible by calculation of all relaxation times: (i) Pressure relaxation time (characteristic of the processes of redistribution of reservoir pressures), which also takes place for thermodynamically equilibrium systems (model LTE—local thermodynamic equilibrium). (ii) Relaxation time of phase transitions, depending on the coefficients of mutual diffusion of the mixture components and the interaction of the mixture with the pore space. The possible effect of the phase transition time, which in the framework of the LTE model is assumed to be negligible, is calculated for the gas condensate system under free volume conditions. Experiments with a model gas condensate mixture in a wide range of thermodynamic parameters were carried out at the Plast facility. The characteristic relaxation time for the boundary and initial conditions taken in the calculations was 700 s. in various experiments, the gas-dynamic time (the time during which a portion of the fluid flows through the experimental site) depending on the conditions is 200–300 s. In the present work shows the necessity of taking into account the relaxation time of the pressure in the development of mathematical models of filtration of fluids with the features on the phase diagram of the mixture.

4. Methods of Mathematical Modeling

Volume-localized excited states in ionized C_{60}

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Due to their hollow highly symmetrical structure and nanometer size fullerenes exhibit appearance of diffuse atomic-like orbitals bound to the molecular core. These SAMOs (superatom molecular orbitals) are electronic states arising from excitation of atomic-like molecular orbitals, in which the electronic density is localized both inside and outside of the fullerene cage [1].
We extend here the previous theoretical results [2], which demonstrate the existence of discrete volume-localized levels in ionized C_{60}. By means of the density functional theory (DFT) we perform precise calculations of fullerene electronic band structure and transition rates between SAMOs and lower unoccupied orbitals. The results of the calculations give us the possibility to get more accurate estimates of the lifetimes of such exited volume-localized states. The possible practical applications of this phenomenon are discussed.

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An extension of a linearized finite-difference model of gas dynamics with the property of entropy non-decreasing to two-dimensional case

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This work continues the research [1]. The new one-dimensional linearized Godunov scheme for equations of fluid dynamics have been proposed in [1]. The main difference from the classical Godunov scheme is that the nonlinear decays of the discontinuity are replaced by its linear analogues, which leads to the shutdown of the iterative process inside the scheme. Earlier, we checked the order of correctness and accuracy of the proposed scheme for simple problems with shock waves. Now we are interested in understanding the internal structure of the scheme and the obtained numerical solutions compared to its continuous ones. That is why we are turning to the numerical confirmation, that developed scheme has property of entropy non-decreasing on discontinuous solutions. We are also making the first proposals on how to extend our numerical scheme to the two-dimensional case. Explosive tests with shock waves and breakup decays are considered. The work is supported by the Russian Science Foundation (grant 17-11-01293) and by the Council on grants of the President of the Russian Federation (grant NSh-5913.2018.1).

[1] Godunov S K *et al* 2018 *J. Phys.: Conf. Ser.* **946**

About vortices in the tube flow of ideal media

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Numerical simulation, which models the evolution of the initial perturbation in axisymmetric subsonic flow of the ideal gas is presented. The undisturbed flow is an axial flow perturbed by azimuthal velocity, or a twist of the flow around the axis of symmetry.
The twist leads to the establishment in the flow of the annular or ball vortex with increasing or decreasing radial axial velocity of the undisturbed flow, respectively.

The use of the modified algorithm for calculating contact boundaries in the finite element complex EFES

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The results of numerical simulation of the destruction of materials and structures with high-speed contact interaction are presented. The calculation of contact interaction and destruction is carried out using a modified algorithm, which significantly improves the performance of the computational complex and allows numerical experiments with real structures with complex geometry.

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Using high-order schemes for modeling heterogeneous systems during loading

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In the paper, we study the waves propagation in homogenized media under loading. The procedure of homogenization carried out in the following ways: (i) by averaging over the volume of each incoming phase [1] and (ii) by linear defining relation, for example Kelvin–Voigt or generalized Zener models [2].
The material is described by a continual approach, within the framework of the Maxwell model. The equation of state for the condensed substance in the Thait form is applied for closure system of conservation laws. The system of conservation laws is approximated by a two-layer time CABARET scheme [3]. Kinematic conditions were assumed at the borders. The ideal mechanical contact was assumed at the contact surface. The splitting method for CABARET scheme is the most convenient to accounting for temperature effects. The Fourier law is added in system of equation. The shock adiabatic of materials were obtained in the course of the calculation. A comparative analysis with experiment was performed. Shock wave attenuation and velocity profiles in a heterogeneous material are obtained. The test was carried out on the tasks of loading the medium with external force and on the problem of shock-wave loading as a result of the impact of bodies.

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About the adequacy criterion of the emissivity model by the experimental data when determining the true temperature of opaque material from the thermal radiation spectrum

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To determine the thermodynamic (true) temperature of an opaque material from the spectrum of thermal radiation, one should choose a parametric model of spectral emissivity so that this model and the required temperature of the material can be considered adequate to the initial experimental data. The possible adequacy conditions are analyzed. As an example, the process of selecting a model based on published experimental data of a tungsten sample heated in a vacuum at a constant temperature is considered.
This message is the result of further development of the work [1].

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Mathematical modelling of heterogeneous media

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The investigation proposes the analysis of models on the description of heterogeneous medium based on various mathematical operations. Within the framework of the approaches proposed, it is possible to track the influence of heterogeneity on the transfer coefficients and the possibility of considering the different behavior of phases in the process, basing on the features presented of the phases. The main investigation methods [1, 2] are the variational method, self-consistent field method and statistical models in the theory of effective modules. The central method is a conditional moment method [3]. The averaged equations with certain coefficients were found by this method as a result of taking into account both the medium as a whole and each phase separately. The microstructure of the medium is shown by both effective and other coefficients obtained by the method of conditional moments and affected different behavior of the phases. This coefficients reflecting the concept of the carrier phase (connected) and the structural phase transition represents the information about the microstructure of the system under study. The condition of critical connectivity of the condensed phase is obtained and followed from the analysis of the effective coefficients.

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Influence of supercooling on morphology of crystalline nuclei forming in metallic melt

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The control of crystallization of metallic glasses and the production of nanocrystallites with desired structural and morphological properties have a great importance for contemporary industries [1, 2]. In the present study the crystallization of model metallic melt at different levels of supercooling is considered by atomistic simulation method [3]. Structure analysis and quantitative evaluation of morphological characteristics of crystalline nuclei are performed for the system at low and deep supercooling levels. Theoretical model is proposed to reproduce the correspondence between a number of particles of crystalline nucleus and its average radius. We found that the evaluated size dependencies of nucleus radius, the radius of nucleus bulk part and the thickness of nucleus surface layer can differ significantly at different stages of the system crystallization. Namely, ramified structures are formed at deep and moderate supercooling levels. The attachment process of particles to the nucleus surface layer occurs unevenly that is reason why nuclei take a ramified shape. At low supercooling levels, a uniform attachment of particles to the surface layer leads to rapid increase of the radius of the nucleus bulk part. Therefore, at low supercooling the nuclei have relatively rounded or smoothed shape. The present results make a significant contribution to understanding of mechanisms of phase transformation in supercooled liquid and glassy systems.

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Surface self-diffusion and bubble diffusivity in bcc metals

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Surface self-diffusion plays an important role in the motion of a bubble in solids [1], but the mechanisms underlying this are still poorly understood. In this work, the diffusion of bubbles (vacancy clusters) with different radii, as well as the self-diffusion coefficients of atoms on the surface of these bubbles are calculated in two representative bcc metals U and Mo by means of classical molecular dynamics modeling. For the surface self-diffusion coefficient computation we use the method proposed in our previous work [2]. The mean square displacement is found for the surface layer atoms that are identified by the Voronoi polyhedron method. The diffusivities of the bubbles are calculated via the nonequilibrium molecular dynamics based on the Nernst–Einstein equation. On the example of small bubbles it is shown that such a method gives correct results. The bubble diffusivities obtained through the direct modelling and predicted by the continual theory [3] with the use of the surface self-diffusion coefficients are compared for different bubble sizes at similar values of the homological temperature.

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Molecular dynamics simulation of the glass transition of a supercooled Zr–Nb melt

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The amorphous states of Zr–Nb alloy were investigated at different cooling rates and various concentration of Nb with the use of molecular dynamics simulations. The calculations were carried out with new embedded-atom method potential with the angular dependence (ADP) [1]. The phase diagram "cooling rate–Nb concentration" and threshold cooling rate for glass transition for the Zr–Nb alloy were obtained. Also, the glass transition temperatures for the Zr–Nb alloy were determined using different criteria. The structure of the amorphous phase was analyzed using radial-distribution function (RDF). It is shown that for zirconium, the splitting of the second RDF peak could not used as glass transition criterion. In addition, the structure was analyzed using the Voronoi polyhedra [2]. In particular, it was found that the number of icosahedral clusters begins to increase sharply during glass transition. This effect can be considered as a glass transition criterion for the Zr–Nb alloy. Moreover, the results of the present investigation are in good agreement with the result obtained by the other authors [3]. All calculations were performed using the LAMMPS package [4] using supercomputer resources of the MSC RAS.

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Simulation of Si–Au nanoparticles crystallization

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Silicon nanoobjects are very interesting for nanophotonics due to unique optical properties depending on the atomic structure. Thus, it is a great interest in study the structural features of these particles, such as the grain size and the distribution of Au atoms in crystal grains and between them. The influence of cooling rate on Si–Au nanoparticles (NPs) structures was studied in this work for different NP sizes and Au concentrations. The simulations were carried out in the quasi-2-dimensional case: one of the sizes in the calculation cell was about 3.5 nm, and periodic boundary conditions were used. This may result smaller grain sizes in simulation in comparison to the experiment. That is why additional one-dimensional simulations were performed to study the grain size dependence on the Au concentration in Si–Au NPs. The movement of the crystal grain boundary and changes in the gold distribution during crystallization were analyzed. The results of simulations indicate that gold atoms try to leave crystallization area via atomic diffusion. So this effect leads to smaller grain size for larger Au concentrations.

The work was supported by the Presidium RAS within the scientific program “Condensed matter and plasma at high energy densities”.

The singularity of the two-particle correlator in the vicinity of the phase transition point of pure metal melt

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The phase transition point of the substance, in spite of its exclusive effect on the behavior of a substance is not special for its thermodynamic functions [1, 2].
It is shown that certain two-particle motion correlators have singularities in the neighborhood of the phase transition point. Correlators similar to those described in the paper [3], were calculated for systems of pure metal melt, modeled by the molecular dynamics method. The time behavior of the motion correlators is different in the liquid stable and supercooled metastable melt phase for a variety of metals. A physical interpretation of such spatial correlations of long-range order in metastable systems is also given. Dependences of correlation functions on the rate of cooling, as well as on the size of the system are also described.
Work has been supported by the grant of the President of Russian Federation for support of leading scientific schools grant NSh-5922.2018.8.

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Velocities relaxation in the Lennard-Jones system

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We present various aspects of the nonequilibrium velocity distribution relaxation to the Maxwellian one for the Lennard-Jones system (LJS). Molecular dynamics method is used for obtaining primary data. We study the dependence of the equilibration rate on the formation of initial spatial distributions of atoms. Relaxation from initial random distributions is a monotonous smooth one. Relaxation from initial crystalline distributions to the equilibrium gaseous state includes a prolonged oscillatory part. Numerical results are approximated by analytical formulas for relaxation time τ by analogy with molecular kinetic theory. The dependences of τ on atoms density and temperature are obtained in the form of power functions. We study the behavior of velocity moments in the process of relaxation of the LJS. The difference between the values found and Maxwellian ones ΔI_n is considered. The dependence of this quantity on time is found. Two time slots are allocated. In both time intervals, this dependence is approximated by $A_n e^{t/\tau_n}$, where t is time, A_n and τ_n are coefficients for moments of order n, which are different for two time intervals. It is obtained that $A_n \sim n^\alpha$. The dependence of τ_n upon n is investigated, τ_n has a finite limit for large n. The level δ^{-1} is introduced. Functions ΔI_n reach this level in time τ_n^δ. It is found that this time grows with n like $\tau_n^\delta \sim \tau_n \ln(n)$. The abstract was prepared within the framework of the Basic Research Program at the National Research University Higher School of Economics and supported within the framework of a subsidy by the Russian Academic Excellence Project '5-100'.

Atomic mechanisms of high-speed migration of symmetric tilt grain boundaries in nanocrystalline Ni

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Molecular-dynamic modeling of structural rearrangement features in nanocrystalline Ni with symmetric grain boundaries of slope (GB) under shear loading was carried out. It was found that GB can be displaced in the direction perpendicular to the direction of shear loading. To activate the displacement, it is necessary to reach the threshold value of the shear stress. The displacement of the GB is abrupt and is due to a certain sequence of displacements of the atomic planes adjacent to the GB. The use of periodic boundary conditions prevents the rotations of the grains. As simulated tilt GB is symmetric, both of the crystallite grains will have the same shear moduli in the direction of the applied loading. Shear loading of crystallite with such a structure does not lead to any volume driving forces. The displacement of GB was entirely due to a coupling effect. Despite the high stress values, the displacement of GB did not cause the nucleation of the defective structure in the simulated crystallite.
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Numerical simulations of impact Taylor tests

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Finite element method is employed for numerical simulation of yielding under dynamic impact Taylor tests. Three different approaches for prediction of plastic deformation of materials are compared with experimental results. These are von Mises, Johnson–Cook and incubation time based yielding criteria. The simulation results have shown that the simplest method based on von Mises plasticity model provides good coincidence with experimental profiles of specimen shape in the course of deformation. The shortcoming is that the correct value of yielding stress is depending on the loading rate and should be known beforehand. The other two approaches also provide reasonable coincidence with experimental results but are much more complicated numerically and require identification of additional model parameters. Thus, if there was a method to predict the value of dynamic yielding stress to be used within von Mises criterion then this simple approach could be the optimal choice for simulation of dynamic plasticity in conditions of Taylor test.

Wave-packet molecular dynamics plus density-functional theory method for nonideal plasma simulations

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A new wave-packet molecular dynamics plus density-functional theory (WPMD-DFT) method is proposed for atomistic simulations of nonideal plasmas and warm dense matter. The method is based on the WPMD approach where electrons are represented as Gaussian wave packets. The electronic exchange and correlation effects are treated using an additional energy term taken from the DFT. This term is calculated by integration over the mesh values of the total wave packet density. WPMD-DFT is meant as a replacement for the antisymmetrized WPMD (AWPMD) method which is more time consuming and lacks electron correlation.

We compare the results obtained by WPMD-DFT, WPMD, AWPMD, classical molecular dynamics and Path Integral Monte Carlo for the internal energy of the hydrogen plasma in the temperature range from 10 to 50 kK and the electron number density from 10^{20} to 10^{24} cm^{-3}. We also demonstrate the ability to handle the simultaneous dynamics of electrons and ions by calculating the electron-ion temperature relaxation. The scalability of the WPMD-DFT method with the number of electrons is shown for CPU and GPU implementations.

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Wave packet molecular dynamic approach for plasma phase transition in warm dense hydrogen

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Despite the fact that hydrogen is the most basic element that makes up most of the universe, its equation of state at high pressures is still an issue. One of these questions is the nature of the phase transition at high pressures and temperatures, at which, possibly, it passes into the conducting state [1].
In this work, we use the wave packet molecular dynamic (WPMD) with the potential of the electron Force Field (eFF) [2] as a tool capable of taking into account the non-adiabatic and non-equilibrium aspects of the plasma phase transition and check the results using density functional theory (DFT).
The results of isochoric heating were obtained for densities of 0.3–0.6 g/cc, which showed the existence of the transition of a vibronic nature, corresponding to the excitation of electrons in H_2 molecules. It is shown that this transition can explain the experimentally observed phenomena: a change in the optical properties and the recent results of the isotopic effect [3], which cannot be described by highly accurate coupled electron-ion Monte Carlo calculations [4].

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Numeric simulation of single pulsed plasma jet capillary discharge with an evaporating wall

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Although pulsed plasma jets are important for various applications (nuclear fusion, propulsion, neutron generator and ion source), the effect of multi-jet interactions remains poorly understood. Numerical simulation for interaction of pulsed plasma jets generated by atmospheric capillary discharge is presented. The plasma source is based on a plasma jet established at the end of a capillary discharge at atmospheric pressure. Interaction between the pulsed plasma jets and the shock wave or contact boundary layer is analyzed. Note that the plasma jet for magneto-inertial fusion must be created in a vacuum environment. Preliminary results on an array of pulsed capillary discharges are presented. Main properties of capillary discharge plasma are discussed.
This work was supported by the Ministry of Science and Higher Education of the Russian Federation (project 13.5240.2017/8.9).

Flow bifurcation transitions of inelastic shear thinning fluids in a channel with sudden contraction and expansion

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Bifurcation phenomena of the non-Newtonian Carreau–Yasuda fluid flow through the channel with the sudden contraction and expansion were studied numerically. To that end, the Navier–Stokes equations of the incompressible fluids were solved using the open integrable platform OpenFoam. It was found that increase in Reynolds number leads to the abrupt change in flow pattern from the symmetric to asymmetric one. The critical Reynolds numbers corresponding to this bifurcation transition were found to depend strongly on parameters of the considered non-Newtonian fluid which are responsible for the non-linear dependence of viscosity on shear rate. The bifurcation diagrams were calculated for different parameters of the Carreau–Yasuda model. It was found that the more fluid viscosity differs from the Newtonian behavior, the smaller the critical Reynolds numbers of the bifurcation transitions are and the longer angular vortices are formed. Moreover, a decrease in the range of Reynolds numbers corresponding to a stable asymmetric flow patterns was observed.

This work was supported by Russian Foundation for Basic Research (grant No. 18-29-17072). The numerical modeling was carried out using the computing resources of Joint Supercomputer Center of the Russian Academy of Science.

Microfibers formation in two-phase fluid flowing in three-dimensional channel with variable cross-section: Numerical modeling

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Numerical modeling was used to study regularities of droplets deformation behavior in two-phase blends of incompatible viscous fluids flowing through three-dimensional rectangular microchannel with variable cross section. The velocity gradient profiles were calculated in the transition regions from the wide chamber to the narrow gap at low Reynolds numbers $\mathrm{Re} \ll 1$. Capillary number and fluids viscosity ratio were varied. The stretching of a single viscous droplet in different zones of the channel were analyzed at different values of capillary number and viscosity ratio of the fluid components. It was found that the most effective elongation of a droplet appears at the entrance to a narrow part of the channel. The calculations were carried out for different values of confinement parameter—the ratio of droplet diameter to the gap thickness. The increase in the confinement parameter was shown to result in the substantial increase in droplet elongation degree. The attention is also focused to microfiber formation in concentrated emulsions.

Diagrams of morphological states of two-phase fluid flowing in the coaxial capillaries

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The results of numerical simulation of the morphological states of two-phase immiscible Newtonian fluids flowing in coaxial capillaries at various flow rates are presented. The state diagrams were derived for different capillary numbers characterizing flow conditions in the inner and outer capillaries. The dripping and jetting modes along with several types of the transient flow patterns were found. In particular, it was shown that the increase in flow rate of the dispersed phase results in the narrowing of the classical dripping mode area on the state diagram as well as expansion of the squeezing dripping mode. The narrowing jetting mode was observed with increase in capillary number of the outer channel whereas the widening jet was found with growing of the relative viscosity of the dispersed phase. The squeezing jet mode was observed at high flow rates of the inner fluid. In this case the jet thickness was shown to approximately equal to the diameter of the outer capillary. Hence, the derived state diagrams represent one-to-one correspondence of flow morphologies of two-phase fluids of different viscosities and flow regimes in the coaxial capillaries.

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Surface tension between charged crystallographic surface and ionic liquid

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Previously, the effect of a qualitative rearrangement of the electrical double layer (EDL) structure in ionic liquid (IL) was observed. The changing of EDL characterized by the dimensionless scale of the surface charge k_{ion} as a ratio between the electrode surface charge density and the theoretical maximum counterion charge density in a closely packed ion monolayer. Taking into account that the interface structure generally related to the value of the surface tension, an abnormal behavior of the surface tension value depending on the surface charge is expected. Therefore, in the framework of molecular dynamics we investigated the influence of surface charge on the value of surface tension. The simulated systems represent the model ionic liquid situated between two model electrodes, where the ions were considered as charged Lennard-Jones spheres. There are two different types of the IL: symmetrical where the cation size is equal to the anion size, and unsymmetrical where the size of two different types of ions is not equal. The surface charge density varies in the range of 0 to $1.5k_{\text{ion}}$. Concentration distributions of ions, electrical potential profiles and one-dimensional distribution of Pn and Pt were obtained. The transition from the multilayer structure to monolayer at $k_{\text{ion}} = 1$ was observed. The oscillations in potential profiles disappear upon $k_{\text{ion}} = 1$. In this case it varies linearly between the surface and the monolayer. Also, it was discovered that surface tension has a minimal value at $k_{\text{ion}} = 1$. Calculations were performed on the clusters MVS-10P and MVS-10Q of the Joint Supercomputing Center RAS.

Calculations of viscosities of liquid hydrocarbon mixtures using molecular dynamics simulations and correlation rules

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The report presents the results of calculations of shear viscosity coefficients for one-component hydrocarbon liquids and binary and ternary mixtures using classical molecular dynamics (MD) method. The MD simulations are performed for the methane–n-butane–n-pentane system with the TraPPE-EH forcefield [1] at the temperatures from 300 to 360 K. The shear viscosity is calculated as a function of density using the reverse non-equilibrium molecular dynamics method [2]. The viscosities of pure liquids are in good agreement with the experimental data available in literature. The simulations show that the viscosity-density dependences for hydrocarbons may be correlated using a form similar to the expanded fluid relations [3]. Mixing rules for the viscosity correlation are proposed and tested. The calculations of mixture viscosities using the mixing rules demonstrate good correspondence to the direct MD simulations results up to the pressures of few hundred atmospheres.

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The viscosity predictions for branched alkanes at pressures up to 1 GPa by molecular-dynamics methods

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Shear viscosity is one of the key subjects of molecular modeling since this quality is used in the development of lubricants [1]. In this work, we use molecular-dynamics methods to predict viscosity dependence on pressure up to 1 GPa for 2,2,4-trimethylhexane. The COMPASS class II force field is used to determine atomic interactions in the model [2]. The shear viscosity is calculated using Green–Kubo and Müller–Plathe methods. To achieve the convergence of the Green–Kubo integral, the time decomposition method [3] is used. The approach is validated by 2,2,4-trimethylpentane for which experimental data are available. The calculated 2,2,4-trimethylhexane viscosity coefficient dependence is fit by Tait-like equation and does not show super-Arrhenius behavior. The predicted values of 2,2,4-trimethylhexane viscosity match the experimental data within the accuracy of the methods up to 500 MPa. The abstract was prepared within the framework of the Basic Research Program at the National Research University Higher School of Economics and supported within the framework of a subsidy by the Russian Academic Excellence Project '5-100'.

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Shear viscosity from diffusivity based molecular dynamics methods

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The molecular dynamics methods for calculation of shear viscosity based on liquid diffusivity (D) are tested against the classical Green–Kubo (G–K) relation for n-pentane at 330 K and 0.601 g/cm^3.
The D-based method shows the same accuracy as well established G–K methods of viscosity calculation. The difference between these results is close to the statistical uncertainty of the simulation.
The Stokes–Einstein ratio gives an accurate result when applying the stick club boundary condition. However uncertainties that arise from the theoretical formulation of this relation are more significant than uncertainties of G–K and D-based methods.
The simulation results are consistent with experimental data. This validates the application of the OPLS-AA force field and the approaches used.
This work is supported by grant No. 18-19-00734 from the Russian Science Foundation.

Continuum modeling of two-phase flows in porous media

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The present work is aimed at modeling flows of natural gas condensate. Phase diagrams of such mixtures contain a retrograde zone. During exploitation it leads to reducing of liquid extraction from gas condensate reservoirs.
In essence, the model is based on [1]. It is isothermal and consists of continuity equations for each component with Darcy's laws for phases filtration velocities. The phases pressures are represented by cubic equation of state [2] and are supposed to be equal. Component flow approach avoids defining of phase transition term. It can be used for mixing and non-mixing fluid in a unified way. The usage of concentrations of components in hydrodynamics equations provides a clear way for modeling mixtures with arbitrary compositions. First results for the flows of binary mixtures are provided.
The research is financially supported by the Russian Science Foundation (project ID 17-79-20391).

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Present and future in heat exchangers design

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Design of heat exchangers (HE) and the methodology of their use have been developing for many years. By this stage, the most widely used tubular and plate HE.
Tubular HE are initially designed and calculated by known engineering, mainly one-dimensional, methods and local effects in them are investigated by CFD (Computational Fluid Dynamics) methods.
The search for optimal forms of plate HE is carried out using CFD methods to obtain the criteria of thermal-hydraulic dependencies in elementary cells and classical engineering techniques to determine the parameters of HE. To validate CFD calculations, experimental studies of representative models of plate heat transfer surfaces of different shapes (corrugated, hilly) are carried out. The choice of surface type is also associated with technological and strength advantages or limitations, such as, for example, the uniformity of the drawing in all directions during stamping and the possibility of spot welding at the contact points of the envelopes of hilly plates.
Additive technologies, which have removed a significant part of the restrictions on the geometric shape of HE, introduce new approaches to the design of heat exchange surfaces and channels. Mutually porous structures and topologically optimal branched tree-shaped heat exchange channels will allow achieve greater efficiency and better weight and size characteristics of HE. Integration of topology optimization software in engineering systems will allow to design HE with branching channels not less effective than, for example, the human circulatory system. In CIAM designed and manufactured according to additive technology perspective branching HE demonstrator with mutually porous structure.

Fully implicit method with lower-upper symmetric Gauss–Seidel preconditioner on multiple graphics processing units for hypersonic flows

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In this paper, we present implementation and benchmarking for gas dynamic solver for hypersonic flow problems with a fully implicit scheme. The aim of the paper is to verify and measure efficiency of the implicit method for multiple graphics-processing-unit computational architecture. The verification is performed on a flow over the sphere-cone problem. We consider hypersonic flow regimes of Mach number M = 20–30. New results are cross-compared with results of the previous version of the code for explicit time marching scheme.

Is a photon a dissipative structure?

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In paper [1], it was shown that the concept of a photon as a dissipative structure arising at the submicroscopic level of a thin medium makes it quite easy to interpret some of the fundamental tenets of quantum mechanics that are still not completely understood in the framework of modern quantum theory. These include, for example, such issues as clarifying the nature of wave-particle duality, the physical meaning of Planck's constant, and also the establishment of a physical law according to which single photons can form monochromatic electromagnetic radiation. Further application of this synergistic approach can also be used for a simple and clear explanation of the polarization of a photon and, following from it, the probabilistic nature of its behavior [2]. For example, it is possible to show this on the basis of the structural-dynamic (vortex) model of a photon adopted by us [1]. Further, on the basis of the previously formulated criterion of the nascence and kinetic stability of the dissipative structure far from equilibrium, the stability and lifetime of a single photon are studied [3,4]. In addition, the topological aspect of electron-positron pair annihilation is considered [5,6].

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Mathematical modeling of helicopter blade icing in flight conditions

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The work is devoted to the problem of correct mathematical modeling of aircraft icing in flight conditions at the stage of preparation for its ground tests. An innovative approach to the solution of this problem is described, which represents the computational and analytical method, tested on the model of the helicopter blade. Mathematical modeling of the blade icing is performed in order to determine the configuration of the equipment and test model on the experimental facility and to identify the most dangerous flight modes in terms of icing, which allows to limit the volume of full-scale tests and thereby reduce their cost. The calculations were performed through the use of modern software packages: ANSYS CFX (the calculation of aerodynamic flow around the model and calculation of droplet flow fields) and ANSYS FENSAP ICE (calculation of mass of ice growths on the surface of the model). The calculations were realized at different operating conditions (speeds, temperatures, liquid water content of incoming flow and angles of attack) with anti-icing system turned on and off. According to the calculated values of the masses of ice growths the list of critical modes is determined. This list is recommended to test the aerodynamic profile. The most dangerous mode is the one in which the mass of the ice growths is maximum. Also, based on the results of the calculations, recommendations on the location of the model on the stand are given and the operating parameters that need to be maintained on the facility for modeling operating modes are determined. The computational and analytical method allows to estimate the icing of the tested model qualitatively in a short time, which makes it possible to significantly reduce the time of experimental research.

5. *Physics of Low Temperature Plasma*

Diffusion in ultracold strongly coupled multiply charged plasma

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We present the results of calculations of electron and ion diffusion by the method of molecular dynamics in an ultracold multiply charged plasma. These calculations were carried out over a wide range of Coulomb coupling parameter. The problems of similarity for a multiply charged Coulomb plasma are discussed. It is shown that in a multiply charged classical plasma for the diffusion coefficients in a wide range of coupling parameter, the similarity assumption is valid. The work was supported by the Russian Science Foundation (grant No. 18-12-00424).

Study of the spectra of calcium-40 Rydberg atoms in magneto-optical trap

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Our research is focused on the laser cooling and trapping of neutral atoms in a magneto-optical trap [1, 2], and study of gases of Rydberg atoms and ultracold nonideal plasma. We have assembled the experimental setup for laser cooling of Calcium atoms. The maximum concentration of atoms in the trap was 2.3×10^9 cm^{-3}, and the number of atoms was 9.5×10^6. The spectra of Rydberg atoms with the principal quantum number $n = 50$–70 were recorded. We used the method of the differential two-photon spectroscopy [3] to estimate the temperature of trapped atoms. The temperature of the atoms in the trap was about 5 mK.

We suggest using a scheme for stabilizing the frequency of laser radiation to create highly excited Rydberg atoms by the spectrum of saturated absorption in a cell with a gas of rubidium atoms.

This work was supported by the Russian Science Foundation under project No. 18-12-00424.

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Plasma phase transition in warm dense hydrogen

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First-order fluid–fluid phase transition in warm dense hydrogen was investigated by different authors both theoretically and experimentally for the last dozen years. The current status of the problem is presented. Arguments pro and contra plasma nature of the transition are discussed. Initial arguments against are: low temperatures about 10^3 K and densities ten times larger than the density of solid hydrogen in the triple point. The new arguments for are: jump from molecular to ionized state at the transition and sloped return form of the isotherm loop. The unusual loop form, drastically different from the van der Waals loop, is specific for plasmas and confirmed by both density functional theory and chemical models. The conclusion is that the experimental results for the transition could be interpreted as an experimental detection of the plasma phase transition. Thus, the prediction of 1968 came true. Another two predictions are confirmed also: a triple point on the melting curve and strong overlapping of the equilibrium and metastable branches for $P(V)$. Structures are observed in the ionized state with interproton distances which are equal to the distances between protons in ions H_2^+ and H_3^+. An analysis of the twin phase transition in solid hydrogen under high pressure allows to reveal the character of the new structure. Five protons form a quasi-tetrahedron consisting of two triangles with a common center. Four distances from the central proton are 0.92 Å, as in H_3^+, and do not change under compression. So, a new feature is a complex cluster composition of plasma formed at the transition. The work is supported by grant No. 18-19-00734 of the Russian Science Foundation.

Metastable conducting solid hydrogen at high pressures

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Density functional theory is applied for the calculation of the equation of state, pair correlation function and conductivity of solid hydrogen. Hysteresis of the dependence of pressure on density is observed. The calculations have been carried out within the density range from 1.14 to 2 g/cm^3 at temperature 100 K. The monoclinic lattice of the C2/c space group, with 24 particles in the unit cell, is used as the initial configuration, since this structure is the most stable in the pressure region above 260 GPa, which corresponds to solid hydrogen phase III at the temperatures under consideration. At the first stage following points are obtained by squeezing the computational cell and relaxation at the constant volume. A structural transition is observed at a density 1.563 g/cm^3. Five protons form a quasi-tetrahedron consisting of two triangles with a common center. Four distances from the central proton are 0.92 Å, as in H_3^+, and do not change with changing density. The value of the distance corresponding to the first maximum of the PCF remains the same in the density range from 1.563 to 1.573 g/cm^3. Following compression of the initial density 1.14 g/cm^3 leads to the structure destruction and formation of the amorphous state. At the second stage structure obtained for the density 1.565 g/cm^3 was used as the initial configuration. Following expansion of the structure showed the stability of the nonmolecular configuration in a density range $\rho = 1.4$–1.8 g/cm^3 and pressures lower than obtained for the density 1.14 g/cm^3. The work has been funded by the Russian Science Foundation (grant No. 18-19-00734).

Density effect: Restriction of atomic excited states at the ionization limit

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Earlier [1, 2], the effects of density and non-ideality were separated for the case of equilibrium collisional electron–ion plasma. Restriction of the concentration of atomic excited states at the ionization limit is the effect of density. It was determined by the concentration of charged particles in electron–ion plasma. Note that the concentration of excited states diverges at the ionization limit in the approximation of an isolated atom. Calculations of a smooth decrease to zero of the concentration of excited states as they approach the ionization limit were carried out and effective lowering of ionization potential was found [1, 2]. The similarity ratio in charge concentration was established. All calculations [1, 2] were carried out for a fixed lifetime of the excited states (the number of electron rotations in orbit in the semiclassical approximation).
In this work, according to the method [1, 2], we calculate a smooth decrease to zero of the concentration of atomic excited states, as we approach the ionization limit, for several numbers of electron rotations in orbit. In combination with the known radiation lifetimes of the excited states, this makes it possible to determine the real dependences of the decrease to zero of the concentration of atomic excited states (their effective statistical weight) as we approach the ionization limit in equilibrium plasma. The work is supported by grant No. 18-19-00734 of the Russian Science Foundation.

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Stopping power and velocity diffusion for a proton moving in a gas of super magnetized electrons

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The first studies of the problem of the exchange of energy of charged particles in a strong magnetic field were related to the idea of electron cooling proposed by Budker in 1966. Derbenev and Skrinsky proposed an approach to determining the force acting on a proton moving through the electron gas in strong magnetic field, as well as determining the velocity diffusion rate for this case.
New interest to the energy exchange problem for charged particles in magnetic field occurred in connection with experiments on antihydrogen. In these experiments antiprotons are injected in the cloud of ultracold positrons. The positrons density is about $n_{\mathrm{e}} \sim 10^8$ cm^{-3} and temperature is about tens of kelvins. In these conditions Coulomb logarithm, which arise due to cross section divergence is small, this fact can break the validity of the Derbenev and Skrinskii approach. Moreover magnetic field is so high that positrons are super magnetized, i.e., gyroradius is much smaller than Landau length e^2/T_{e}.
The current work is devoted to calculation of energy exchange rate for a proton propagating through the electrons gas in strong magnetic field for conditions similar to those in the experiments on antihydrogen. Validity of Derbenev and Skrinsky theoretical approach is checked for low values of Coulomb logarithm. Calculations were made for high proton velocity as well as for low velocity when the theoretical approach has logarithmic divergence. The reported study was funded by the Russian Foundation for Basic Research according to project No. 18-32-00421. The calculations were performed at the Joint Super Computer Center of the Russian Academy of Sciences.

Angular dependences of s- and p-polarized reflectivities of partially ionized dense plasma

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For further development of nonideal plasma physics, investigations of its electronic subsystem properties appear to be crucial. The correct description of collision processes in a dense partially ionized plasma is possible only on the basis of sufficient information about the transport properties of the such medium. Studies of the optical-polarization properties of explosively driven dense plasmas using the technique of inclined probing can provide the required physical information.

The results of new experiments on reflectivity of polarized light on nonideal xenon plasma are presented. The measurements of polarized reflectivity coefficients of strongly correlated dense plasmas have been carried out at incident angles up to $\theta = 70^\circ$ simultaneously for s- and p-polarization using laser light of frequency $\nu_{\text{las}} = 2.83 \times 10^{14}$ s^{-1}. The plasma composition was calculated within the chemical picture [1]. During the experiments, the plasma density $\rho = 1.8$ g/cm^3, pressure up to $P = 10$ GPa and temperature up to $T = 32000$ K were realized. Under these conditions, the plasma is non-degenerate.

The new experimental points are used in the integration of corresponding Maxwell equations to construct the spatial profile of the density of charge carriers. A simple model of the ionization kinetics of the plasma transition layer is considered.

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Metallization effect in shock-compressed inert gases

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Under shock-wave compression of condensed inert gases, an abrupt (depending on density) increase in conductivity was observed in experiments [1]. When compressing inert gases, initially in the gas state, a high conductivity was observed, but it is weakly depending on the density. In this work, the previously proposed "3+" model [2] is applied to the calculation of the dense inert gases conductivity taking into account their specificity. Inert gases are fundamentally different from metal vapors. In the gas state, they are dielectrics and remain so during cooling and compression up to the liquid and solid states. The use of the proposed in [2] method of the jellium density calculation leads to its appearance in the compressed rare gases. The resulting jellium should be considered dielectric because it arises from a fully filled electron shell. Jellium electrons do not give the direct contribution to the conductivity and the collective binding energy of atoms. A new, unusual for plasma physics effect associated with the broadening of the ground level of the atom due to the formation of jellium in the equation of ionization equilibrium is proposed in this work. The appearance of such a broadening will facilitate thermal ionization, bringing the energy of the ground state of the bound electron to the continuum, acting as a kind of lowering of the ionization potential, but on the other side of the energy scale. The composition and conductivity of dense, ionized inert gases are calculated. It is found that the account of the broadening of the ground state caused by the appearance of jellium leads to a quantitative agreement with the experimental data. We can talk about the semiconductor nature of conductivity.

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The thermophysical properties of low-temperature carbon plasma

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The thermophysical properties of a substance (the pressure, the internal energy etc. and the electronic transport coefficients) can play crucial role for various fundamental tasks and applications. Presently there are even the data for the low-temperature plasma of some metals [1] at the temperatures $T = 10$–100 kK. For carbon there are also corresponding measurements [2–4] and calculations [5–7]. But at relatively low densities, for instance below 1 g/cm^3, there are only the data for the electrical conductivity. The data on the pressure and the internal energy as well as for two other coefficients—the thermal conductivity and the thermal power—have been absent up to now. This is the reason to developed a model to close this gap [8]. We have calculated the considered properties for the low temperature carbon plasma and compare our results with the data of other researchers, where available, including the most recent calculations [9].

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Comparison of the properties of plasma and nanoplasma by the example of the thermionic emission model

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Nanotechnology and interaction of intense energy fluxes with matter are two very popular and at the same time very different areas of research. However, there is the natural intersection of these disciplines. It aims to answer the following questions: What happens if the nanoscale object is irradiated with intense laser pulses? The result is the nanosized object with a relatively high electron temperature density and degree of ionization. It's called nanoplasma.
This paper presents a theoretical model of emission current from nanoplasma. The model consists of a system of ordinary differential equations. Comparison with a series of experiments [1, 2] is presented. The suggested system of equations allows generalizing the experimental results and giving a new explanation of some of them. The work pays special attention to the differences between plasma and nanoplasma.
The abstract was prepared within the framework of the Basic Research Program at the National Research University Higher School of Economics (HSE) and supported within the framework of a subsidy by the Russian Academic Excellence Project '5-100'.

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Low bond viscosity limit for strongly coupled systems under shock wave loading

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Shear viscosity measures how disturbances in the system are transmitted to the rest of the system through interactions. Thus low shear viscosities indicate significant interaction strength [1]. Nature of low bond viscosity limit represents general interest in physics of condensed matter and high energy physics to qualify properties of scattering area that separates different phases of matter constituents under extreme loads [2, 3]. Defects and collective modes being by the nature the local and global symmetry breaking were introduced as gauge field and string objects related to specific type of critical behavior—structural-scaling transition. Original shock wave experiments for metals and fused quartz supported the links of scattering effects at shock wave fronts, low bond viscosity and anomalous relaxation due to the "subjection" of critical (metastable) system to the set of collective modes of defects. Transformation of solitonic waves into the blow-up structure in shocked quartz at failure wave front provides the low viscosity limit and is considered as the acoustic scenario for black hole phase transformation. Systems with strong coupling (classical one as fused quartz and strongly coupled plasma) have a small viscosity as compared to weakly coupled plasmas in which the viscosity is proportional to the mean free path [4].

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Betatron oscillations, synchrotron radiation and emittance of electron bunches accelerated in guiding structures

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Wakefields generated in guiding structures (plasma channels and capillary waveguides) by laser pulses can be effectively used for acceleration of electron bunches to high (from GeV to TeV) energies at short (in comparison with usual linear accelerators) length in the process of multistage acceleration, and also for creation of compact sources of short-wavelength synchrotron radiation. Controlling of betatron oscillations is crucial both for ensuring sufficient quality (i.e. low emittance, low energy spread and high number of trapped and accelerated particles) of electron bunches during acceleration and also for other use of accelerated bunches for effective generation of synchrotron radiation.
The related processes of betatron oscillations, synchrotron radiation and dynamic of emittance [1, 2] of electron bunches accelerated in plasma channels and in capillary waveguides are studded theoretically and with the help of numerical simulations. Possible approaches for control of emittance and synchrotron radiation of electron bunches are discussed.

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Momentum distribution functions in quark–gluon plasma

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Based on the composite quasiparticle model of quark–gluon plasma (QGP), the Wigner function is represented as an integral of the color path. The Monte Carlo calculations of the quark and gluon densities and the momentum distribution function for strongly coupled QGP plasma in thermal equilibrium at barion chemical potential equal to zero have been carried out. Comparison with Maxwell–Boltzmann distribution shows the significant influence of the interparticle interaction on the high energy asymptotics of the momentum distribution functions resulting in appearance of quantum "tails".

Thermodynamics of the Debye liquid

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The thermodynamic potentials of charged dust particles interacting by the Yukawa potential were studied using the Ornstein–Zernicke integral equation of a fluid and the method of Brownian dynamics. The methods of closure of the correlation functions on the basis of the hypernetted-chain (HNC) equation and the Percus–Yevik (PY) approximation are considered. The internal energy, free Helmholtz energy, entropy and isothermal compressibility of a fluid are calculated, the latter two values being calculated by two different methods. The effective nonideality parameter Γ^* varies from 0 to 155 and the structure parameter κ from 1 to 5. It is considered the cases when the screening constant is a function of temperature and not depends on temperature. It is shown that the values of the free Helmholtz energy in these two cases turn out to be very close to each other, although the values of the internal energy noticeably differ. Comparison of these calculations by the method of fluid integral equations with those calculated by the method of molecular dynamics showed that the HNC equation turns out to be sufficiently accurate to calculate the thermodynamic potentials of the Debye fluid, and the PY approximation turns out to be a rather rough approximation.

Also, a dusty plasma was considered as a multicomponent system of charged particles, the interaction of electrons and ions with electrons, ions and dust particles was considered in an ideal approximation, and the interaction of dust particles with each other was considered on the basis of the Ornstein–Zernike equation in the HNC approximation. The pressure, free Helmholtz and internal energies, and the isothermal compressibility of a multicomponent system as a function of the nonideality parameter and the structure parameter are determined.

Rotation of the dust structure in the region of the narrowing of the dc glow discharge current channel in a strong magnetic field

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It is known that dust structures in the strata of a dc glow discharge rotate when a longitudinal magnetic field is applied. With increasing magnetic field B the direction of rotation changes; at low fields ($B \lesssim 0.01$ T) the magnetic induction and angular velocity vectors are oppositely directed, at strong fields ($B \gtrsim 0.1$ T) they are unidirectional. To form standing strata and stabilize the cathode spot, narrow discharge diaphragm with a hole 5 mm in diameter were placed in the discharge tube near the cathode. In the area of narrowing of the channel, a trap for dust particles occurs, where the dust structure is formed. This structure also rotate in magnetic field, however we have not observed the rotation inversion. At any magnetic fields up to 1 T, the field and angular velocity are oppositely directed. Based on the theoretical approach developed by us earlier we estimated the rotation velocity of the dust structure in this area and obtained qualitative agreement with the experimental data.

Experimental study of the wakefield behind a dust particle in the He–Kr direct current discharge

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Experimental study of the wakefield behind a dust particle in a dc gas discharge containing an easily ionized impurity of heavy atoms was performed. The main buffer gas was helium (He); inert krypton (Kr) was used as an impurity. During the experiment, the molar amount of impurity in the gas mixture ranged from 0 to 2.4 vol %, while the pressure of the gas mixture was maintained at 50 P. Two monodisperse polystyrene particles were suspended under each other in a stratum of the positive discharge column. Video recordings of dust particle trajectories made it possible to study the interaction between dust particles, as well as the external electrical forces acting on the particles from the discharge. We found that a small fraction of the impurity of heavy ions in the plasma of a light gas significantly affects the wake structure which is formed due to the perturbation of the ion flux by the charged macroparticle.

Effect of the non-linear screening on thermodynamics of complex plasmas

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The so-called "Debye–Hückel plus hole" approximation [1] was modified when the non-linear screening effect is taken into account in a highly asymmetric complex plasma of macroions and microions. Parameters of the non-linear screening of the macroions were obtained within the framework of the Poisson–Boltzmann approximation [2]. Two effects are found as a result of such calculations: (i) subdivision of all microions into two subclasses, bound and free ones, and (ii) significant reduction of an effective charge Z^* of the macroion in comparison with its true value Z due to the appearance of a thin high-density envelope of the bound microions around the macroions. The value of Coulomb interaction energy differs considerably in the case when the non-linear screening is taken into account.

Free energy of a mixture of two sorts of macroions with charge numbers Z_1 and Z_2 was estimated within the Wigner–Seitz cells approximation. The non-linear screening effect was taken into account via the Poisson–Boltzmann approximation within the both cells. The equality of microions pressures at the boundary between cells with the different sorts of macroions was used as an equilibration condition.

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Correlation-driven anomalies in screening charge profiles in highly asymmetric complex plasmas

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It is well-known that the screening of macroions (with the charge Z) by microions in a strong asymmetric ($Z \gg 1$) complex plasma at low temperatures ($kT \ll Ze^2/D$) differs significantly from the linearized Debye–Hückel screening in two aspects: (i) non-linearity of screening already in correlationless Poisson–Boltzmann approximation (Martynova-2018); (ii) "squeezing" of the microions screening claud due to ion–ion correlations (Iosilevskiy-1985) (Chigvintsev-2018). Present work deals with the latter effect. To calculate a profile for screening microions, a variational approach in local density approximation is used. The microions are described as classical charged hard spheres of diameter d with a local EOS (Chigvintsev-2018) that takes into account microions correlation ("non-ideality"). As it was claimed previously, e.g. (Iosilevskiy-1985) a direct non-ideality effect in local EOS is the appearance of phase transitions at low enough temperature, that results in turn the gaps in profile of screening micro-ions, which separates in this case into a dense "liquid" layer (and/or "crystal" shell) stuck to a macroion, and a diffuse "atmosphere" far from it. The characteristics of this separation of all micro-ions into "free" and "bound" ones and the effective ("visible") charge of the macroion $Z^\star$ ($Z^\star \leqslant Z$) are calculated. The results are compared with the data of similar subdivision obtained in the Poisson–Boltzmann approximation (Martynova-2018).

Electric field influence on dust particle dynamics in dust vortices

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We study dust vortices called dust devils and dynamics of dust in this structures. Dust devils are well formed relatively short-lived vortices that can appear over well heated surfaces like deserts and are clearly visible due to large amount of dust raised. Dust particles rotating in a flow bump and scrape each other and as a result particles obtain electric charges. Space separation of particles with opposite charges leads to generation of macroscopic electric field. We simulate dust dynamics with taking into account the electric field of the vortex. The work is supported by the Russian Scientific Foundation (project No. 18-72-00119).

On dusty plasma formation in Martian ionosphere

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A self-consistent model for the formation and evolution of dusty plasmas in Martian ionosphere is developed. The effects of the initial distributions of dust particles, as well as condensation and absorption of carbon dioxide and water molecules by dust particles, are studied. Theory values of characteristic sizes of dust grains and their charges are obtained. The theoretical values of the sizes are in agreement with the data of observations. The possibility of the formation of dusty plasma structures in Martian ionosphere which are analogous to noctilucent clouds in the atmosphere of the Earth is discussed. This work was supported by the Russian Foundation for Basic Research (project No. 18-02-00341) and was carried out as part of the Russian Academy of Sciences Presidium program No. 28.

In situ investigation of the surface of the atmosphere-less space body as the dusty plasma source

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The atmosphere-less space body surface is solarized by the directed ionizing influence in the case of low magnetic fields. Many countries have plans of the exploration of the Moon, the Mars, the Fobos and other space bodies including dust investigation on the surface. It was confirmed for laboratory modeling that the dust particles have levitated in case of simulations close to the real environment of the atmosphere-less space body. The particles populations ($\sim$ 1 μm) may be created on the orbits of Mars satellites and above the Moon surface because these bodies are bombarded by the micrometeoroids, the solar wind and other ionizing rays interaction as well as the acceleration under surface electrostatic fields. In the case of the small space body or the asteroid, where one can have a local magnetic field or some degassing process like comets, etc, the interaction can be significant for creating the dusty plasma environment around the atmosphere-less body. The inventory of instruments must ensure possibility for monitoring the environment parameters such as the measuring ions flows solar wind, the casualty effect for the space rays and the electromagnetic characteristic of dusty plasma. Such instruments complex is allowed to take in the hand the sync information about time-space process of the dust particles behavior and the check of many modern theoretical models.

The effect of amplitude instability onset on the mass transfer processes and the dynamic properties of a two-dimensional Yukawa cluster

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The conditions for the appearance of amplitude instability in a two-dimensional cluster system of Yukawa consisting of seven particles are studied for the case of sufficiently large thermal displacements of particles. We produced a series of Langevin molecular dynamics simulations varying parameters for interparticle interaction and parameters of surrounding media. Our numerical simulations have shown drastic changes in structural and dynamical properties of the system near the critical value of the coupling parameter Γ_c. The investigation of mass transfer processes allowed to determine Γ_c with better accuracy in comparison to methods dealing with the pair correlation functions, or the dynamic entropy. The comparison of Γ_c with the original analytical assessment gave good agreement. We also obtained that there is an obvious general correlation between the conditions for the amplitude instability onset in a hexagonal cluster and the melting criteria for spatially homogeneous two-dimensional systems having primitive hexagonal packing.

Flow formation in monolayer dusty plasma structures under laser action

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The results of an experimental study and analysis of the structures of particles with a dust stream in a plasma of a high-pressure capacitive discharge of low pressure under the influence of a laser are presented. The formation of a flow in the dust structure formed by melamine-formaldehyde particulates was of a threshold nature. When the power of the forcing laser radiation reached a critical value of W_k, a deformation of the structure was observed, but the flow did not appear. With a further increase in the power of laser radiation, the formation of a directed motion of dust particles in the area of the laser beam exposure was observed. It was found experimentally that the value of the laser power W_k, causing the formation of a dust flow, depended on the correlation degree of the dusty plasma system. So with an increase of coupling parameter Γ^*, a decrease in the threshold value W_k was observed. In dusty plasma structures formed by copper-coated particulates, the variation of the power of the forcing laser led to a kinetic heating of the dusty structure, first in the laser-induced region, and later in the peripheral regions of the structure. There was no clearly observable flow channel in the structure. However, the distribution of the particle velocities at different values of the power of the forcing laser showed an increase in the velocity component directed along the beam.

Kinetic temperature and diffusion coefficient in a quasi-two-dimensional system of interacting dust particles at directed external influence

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Quasi-two-dimensional dusty plasma systems are a unique object for studying transport processes and phase transitions at the kinetic level. The simplicity of experimental observation and the ability to control the parameters of interaction and the character of the motion of particles in these systems makes them the subject of numerous studies. In this work, the Brownian dynamics method was used to study the effect of directed external action on a limited region of a two-dimensional system of charged dust particles for various values of the non-ideality parameter of the unperturbed system. It has been found that an increase in the magnitude of the external force leads to an increase in the intensity of diffusion processes and the kinetic energy of the chaotic motion of particles in the region of influence. It has been also shown that the kinetic temperature of the particles has a slight increase in the zone where there is no external effect. The diffusion coefficient in a system of particles calculated from modeling data depends not only on the chaotic component of their velocity, but also on the arising velocity of translational motion of individual particles in different directions.

Moreover, the occurrence of this translational component of the motion of individual particles is most pronounced with the maximum value of the non-ideality parameter of the original system. Thus, for the correct determination of the diffusion coefficient in a system of particles with an external influence, it is necessary to analyze the motion of each individual particle.

Scenario of phase transitions in quasi-two-dimensional dusty plasma systems

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Today, there are two main theoretical models describing melting in two-dimensional systems. According to one of them, the so-called theory of Berezinsky–Kosterlitz–Thouless (BKT), the transition of a two-dimensional system from a crystalline state to a liquid state is of a two-stage nature with the formation of an intermediate phase. Another well-known GBI theory (grain-boundary induced melting) describes the melting of two-dimensional systems as a phase transition from a crystal to a liquid without the formation of any intermediate phase [1–3]. This work is devoted to an experimental study of the phase transition in a monolayer dust structure with its partial heating. The experiments were held in the gas-discharge vacuum chamber. Since the experiment was conducted with the discharge parameters unchanged, the interaction between the particles remained the same, and the kinetic energy increased, a phase transition could have been observed. For this, it was necessary to analyze not only the pair correlation functions, but also the mutual concentration of defects in the structure, since another criterion of the BKT theory scenario is the fact that the phase transition occurs with the formation of free disclinations and dislocations. While the compensated dislocation pairs do not distort the crystal lattice, the free ones do. Hence, analyzing such a system, we can make a conclusion about the phase transition scenarios.

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Wave techniques of dusty plasma diagnostics

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Dusty plasma contains a portion of charged microparticles in addition to electrons and ions. The dust fraction expands the physical properties of the plasma, such as the density of various types of charged particles (including their profiles in an inhomogeneous configuration), the shape and position of the layers in a glow discharge, etc.The fundamental importance of dusty plasma research includes the concept of active particles, gas discharge physics as well as plasma wave physics. In addition, the studies are important from a technological point of view. Despite the large number of works on this topic, the question of accurately determining the parameters of dusty plasma and glow discharge as a whole remains open. It becomes especially relevant in experiments on cryogenic discharge carried out in bulky thermostats and in conditions of a lack of available instruments. In these and other cases, new plasma diagnostic methods are needed. In this paper, the techniques of dusty plasma diagnostics based on the analysis of dust-acoustic nonlinear waves and solitons are developed. As you know, the lower limit of the frequency range of the field-acoustic waves is in the region of 1–100 Hz, and the fluctuations of the dust density by a nonlinear wave are easily recorded with the help of video cameras. On the other hand, the connection of plasma parameters with wave parameters is determined by many theoretical models. The techniques developed are designed to determine the Debye radii, ion temperatures, drift velocities, etc. There is no need to use probes, lasers, external fields that affect the plasma in the diagnostic process.

Dynamics of motion of particles with a modified surface in a plasma–dust monolayer

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The investigation of phenomena associated with phase transitions in plasma–dust structures of active Brownian particles is an urgent task that allows us to study the evolution and self-organization of strongly non-ideal systems. The results of an experimental study of the nature of the movement of melamine-formaldehyde (MF) particles with a modified surface in a plasma–dust monolayer upon exposure to laser radiation are presented. The experiments were carried out in a plasma of a capacitive radio-frequency discharge. MF particles (10.6 μm in diameter) were injected into the plasma and formed monolayer. Based on the data obtained, measurements of the mean square displacement, linear displacement along and across the velocity vector of moving dust particles were carried out. A crystal–liquid phase transition in the monolayer was experimentally observed after exposure in plasma. An explanation of the phase transition is proposed, taking into account the role of photophoretic force in the movement of particulates [1]. It was established experimentally that particles with a modified surface are active Brownian particles and their activity increases with increasing power of the acting laser radiation. It was found that the dynamics of the movement of modified particles change at different laser radiation powers and corresponds to three modes: trap hold, Brownian motion and combined self-motion, consisting of laser-induced (photophoresis) and Brownian motion.

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Dynamics of motion of Janus particles in the plasma–dust structure under external influence

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The study of collective phenomena in systems with active particles has become one of the most interesting and rapidly developing new directions in the physics of soft condensed matter, as well as in the field of statistical mechanics and materials science. This work is aimed at studying the nature of the motion of Janus particles in a dusty plasma structure under external influence. The experiments were held in the plasma of a capacitive radio-frequency discharge. Argon was used as the plasma-forming gas. Janus particles were injected into the plasma and formed plasma–dust structure. The plasma–dust system was illuminated by laser radiation with various power values. Melamine-formaldehyde particles (9.65 μm in diameter) partially coated with metal are used as Janus particles. Based on the data obtained, measurements were made of the mean square displacement, linear displacement along and across the velocity vector of moving particles, and the trajectories of the motion of the particles were constructed. The data obtained allow us to describe the kinetic properties of Janus particles in a plasma–dust structure. It was established experimentally that Janus particles are active Brownian particles and their activity increases with increasing power of the acting laser radiation. It was found that the dynamics of the motion of modified particles change at different laser radiation powers and corresponds to two modes: Brownian motion and combined self-motion, consisting of laser-induced (photophoresis) and Brownian motion.

Particles behavior in alternating corona discharge of quadrupole trap

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Particles dynamics inside alternating corona discharge electrodes of the trap was studied. Four electrodes were mounted parallel to each other at the corners of a square. At the electrodes prebreakdown alternating voltage was applied with phase π at neighboring electrodes. Uncharged aluminum oxide microparticles were injected between the electrodes where they start gaining charges in alternating corona discharge. The frequency of the alternating voltage was 50 Hz and the strength of electric field was up to 30 kV/cm. Using the distribution of electric field and concentration of ions in corona discharge (positive and negative) the particle charges were calculated at every moment of simulation. Analyzing particle motion the areas of particle capturing (the geometric area, parameters of voltage and the geometry of electrodes) and the dynamics of charge change were found.

Solitary waves in a long structure of charged dust particles in linear electrodynamic trap

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The work demonstrates the appearance of a density wave in the form of a single hump in a quadrupole electrodynamic trap in air under normal conditions, when the energy losses due to air viscosity can be compensated by the energy contribution of the altering electric fields of the trap. We have shown that the generation of density waves is possible by adding charged particles to the electrodynamic trap, as well as at smooth increasing the voltage amplitude on the electrodes. The physical mechanism of this phenomenon is the nonuniform velocity distribution of dust particles. A qualitatively agreement of the numerical and experimental results has been demonstrated.
This work has been carried out under financial support of the Russian Foundation for Basic Research via grant No. 18-08-00350.

Calculation of thermodynamic properties of a structure of charged microparticles in electrodynamic traps

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By combining the brownian dynamics and statistical theory of liquid state, the thermodynamic properties of a strongly coupled Coulomb structure in the linear Paul trap were calculated. In particular studying of time evolution of internal energy, pressure, coupling parameter and pair distribution functions of the Coulomb structure have been carried out.

Quadrupole electrodynamic trap as a tool for cleaning dusty surfaces

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This work is devoted to the experimental and numerical investigations of the possibility of cleaning dusty dielectric surfaces using an electrodynamic trap. We used a linear quadrupole Paul trap and polydisperse aluminium oxide particles in our experiments. Numerical simulations were performed using molecular dynamic methods. The phenomenon of lifting and trapping of uncharged particles placed on the glass substrate located under the trap was experimentally observed. The parameters of the trap and charges of dust particles, which are necessary for drawing them from the substrate and confining in the trap, were also estimated using numerical simulations.

The work was supported by the program of fundamental research of the Presidium of the Russian Academy of Sciences "Condensed matter and plasma at high energy densities".

Melting of dusty plasma structures in a trap

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Phase transitions and instabilities in a dusty plasma are of interest to modern physics because of the possibility of direct observation. However, after 25 years of research, the theory of phase transitions in a plasma with dust particles has not been developed, and in most cases the phase diagram of this system is connected with the diagram of the infinite Yukawa system [1].
This work is devoted to dusty plasma in the conditions of a glow discharge. The system is considered in the form of N like charges, interacting by the Yukawa potential and confined by the parabolic trap. Molecular dynamics simulations of this system are conducted at different temperatures of the Langevin thermostat for different values of screening parameter. The temperature of melting is defined from the value of average Lindemann parameter which is supposed to exceed 0.15 after melting.
It is shown that melting of finite Yukawa balls starts at significantly lower temperatures than in case of the infinite Yukawa system. Moreover, the more particles there are in the structure, the lower the temperature of melting start falls. The process of melting starts at the surface of the structure and moves gradually into its center with the increase of temperature. Obtained results allow to explain the mechanism of a phase transition observed in [2] using the theoretical approach developed in [3].

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Charge of a single grain and the grain in a cloud: Theory and experiments

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The effect of cloud density on grain charge is important for complex plasma physics. The quasi-neutrality condition brings about changing of ratio of a space-averaged ion density to electron density in the dust cloud. Strong interaction between ions and highly charged grain complicates the analysis of the effect of ion density increasing on ion flux on the grain. The theoretical approach to ion flux correction on the grain space charge are discussed. The experimental measurements of charges of solitary grains and the grains in the cloud under similar plasma parameters are presented.

Radial confinement of dense dust structure in neon dc discharge at 77 K

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The plasma–dust trap parameters in neon dc discharge at room and cryogenic temperature have been simulated. The simulations were based on the diffusion–drift model of the uniform glow discharge positive column with dust particles developed previously [1]. At room temperature in neon dc discharge of a few centimeters in diameter, the dust structures were formed from individual dust particles, with number density less than 4×10^{11} m^{-3} [2]. With decreasing temperature, the individual dust particles formed clusters [2], which then formed dust structures with a high average number density of dust particles about 10^{13} m^{-3} at cryogenic temperature. The dust particle confinement in the potential trap in a radial direction was determined by potential energy, which at room temperature, was mainly, determined by the action of the radial electric field force, thermophoretic force and ion drag force. To describe the dense dust structures formed by clusters the model assumed that the ion drag force was proportional to the distance between the dust particles in the cluster if the distances were smaller than the Debye ion radius. It was found that in super dense dust structures formed at cryogenic temperature, there was an inversion of the radial electric field, of the electric force and the ion drag force. It was found that these forces form a potential trap for the ordered complex dust clusters [2] in the center of the discharge with a radius close to that observed in experiments. The work is supported by the Russian Foundation for Basic Research, grant No. 19-02-00454.

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The chemical potential of the dust sphere in the cryogenic plasma at a phase transition

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In this work, the self-organization parameters of dust spheres formed in a glow discharge of a direct current in neon at a temperature of 77 K were determined. The composition, phase and dynamic state of the components that form the dust spheres were also investigated. The radial distributions of the potential energy of a dust particle in a glow discharge with dust spheres and an analogue of the chemical potential of a plasma–dust system [1] have been calculated. A change in chemical potential indicates a change in the composition of the mixture of components in a plasma–dust system. It was found that the maximum of the analogue of the chemical potential of a dust sphere corresponds to the minimum of the dust sphere size and is located to the left of the "liquidus" line between the pressure corresponding to the minimum of a dust sphere radius, and the pressure corresponding to minimum of dust sphere current and the potential energy of the dust particle. These minima are located in the region of pressures and currents, where a continuous phase transition occurs in a multicomponent multiphase mixture of complex and simple clusters. It was found that the transition from the maximum value of the analogue of the chemical potential and the subsequent decrease it value at the intersection of the "liquidus" line completes the process of melting of complex clusters and is accompanied by a transition from a multicomponent multiphase mixture of complex and simple clusters to a single-phase homogeneous composition in the form of simple clusters in a liquid state. The study was supported by the Russian Foundation for Basic Research, grant No. 19-02-00454.

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Influence of dust particle number density on the thermophoresis in dusty plasma

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Studies of the formation of dust voids provide a key to detecting the main forces acting on dust particles in a plasma. With the increasing Joule heating of a discharge, the thermophoretic force can play an important role in formation of a void. In [1] the boundary line of a transition of continuous to hollow dust structures, in coordinates gas pressure–discharge current, has been experimentally obtained in a glow discharge in neon. The experiments have been carried out for spherical particles of 2.55 and 4.14 μm in diameter. The simulation of the transition line has been carried out using the diffusion-drift model of the positive column of glow discharge in neon [2], taking into account the radial temperature gradient. It was found that the thermophoretic force acting on particles in a dust structure depends on a discharge parameters and on the sizes of dust particles and dust structure. In this study, have been simulated the boundary line of a transition to void in hollow dust structures, for different values of dust particle number density in a dust structure. The thermophoretic force have been shown to depend on the distance between dust particles in a dust structure.

The work was supported by the Program of basic research of the Presidium of the Russian Academy of Sciences "Condensed matter and plasma at high energy densities".

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Thermal mechanism limits of electrical breakdown of conductive water in terms of conductivity and applied voltage

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It was previously established that the development of an electrical discharge in conductive water is possible at least by two different mechanisms: thermal, with a characteristic channel propagation speed at the level of ten m/s, and streamer-leader with speeds at the level of units and hundreds of km/s. Preliminary experiments have shown that it is possible in principle to implement both mechanisms in water with a fixed conductivity and a change in the amplitude of the applied voltage, i.e., for a given conductivity, there is a certain threshold voltage at which the transition from the thermal mechanism to the streamer-leader mechanism occurs. This phenomenon was explained based on ideas about streamer propagation as an ionization wave. The possibility of streamer propagatioin in a conductive environment is limited. If the rate of diffusion of the potential at the head of the channel exceeds the speed of channel propagation, then the further development of the discharge becomes impossible. Based on these considerations, a theoretical limit was established, dividing these two mechanisms on the voltage–conductivity plot. This work is devoted to experimental verification of the established boundaries.

Anharmonic oscillations of the single dust particle trapped in a standing striation

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The nonlinear forced oscillations of a single dust particle trapped in a standing striation are investigated. The method of the discharge current modulation [1,2] is used to obtain the multiresonance curves at pressure $p = 0.16$ Torr. The frequency responses are investigated depending on the value of the modulation depth. In this paper the parametric instabilities, which were previously observed under the conditions of rf discharge in papers [3, 4], are investigated under in dc plasma. The detailed measurements of the amplitude-frequency characteristic near resonances at the fundamental and doubled frequencies make it possible to detect the vibrational hysteresis.
The theory of the unharmonic oscillator provides a good quantitative description of the experimental data. The values of the thresholds of excitation of parametric instabilities, the unharmonic coefficients and the critical values of the oscillation amplitude for the hysteresis were calculated. The potential energy curve were calculated using the values of unharmonic coefficients.
Work was supported by the Russian Foundation for Basic Research, grant No. 18-32-00685.

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On the mechanism of modification of melamine-formaldehyde particles in dusty plasmas

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Plasma glow and rf discharges of inert and molecular gases is widely used to modify the surface of polymeric materials. In a number of works modification of spherical dust particles of melamine formaldehyde in complex plasma has recently been discovered and quantitatively studied. The method of scanning electron microscopy was used to determine the reduction in the size of particles and the change in the structure of their surface depending on the residence time in the plasma. This report discusses possible particle modification mechanisms. The key issue in the interpretation is how ions having a low thermal energy of 0.03 eV in a low-temperature plasma cause a significant modification of dust granules, since the effect of an electron beam with energies 1000 times greater than that of electrons in the plasma, does not reveal any modification.
Numerical estimates show that the mechanism of modification of particles in a complex plasmas is the action of an ion flow, which continuously goes onto the particles in the process of maintaining their stationary charge. This is consistent with the time dependence of the heating of the material of the particles with the existing balance of energy on the surface of the particle. In addition, heat heating of melamine-formaldehyde has a certain role in reducing particle size. The detected effects can be used for the all-round precision treatment of polymer powders and changes in their surface properties.
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The influence of a magnetic field on the geometrical dimensions of dust structures in striations

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When a magnetic field is applied to a glow discharge, the fluxes of plasma particles redistribute, which in turn can lead to a change in the charge of dust particles levitating in the striation. In this case, a change in its geometric shape and internal ordering of the particles takes place in the dust structure.

In the work, the research of the impact of magnetic field on dust structure created in the striation of the glow discharge is presented. A change of the geometrical sizes of dust structure depending on magnetic field is revealed and also the change of interpartial distance is investigated. The dependence of particles density in the section which is perpendicular to magnetic field depending on the value of magnetic induction is obtained. The schedule of dependence is compared with dependence of angular velocity of rotation of dust structure on magnetic field in three ranges of magnetic field. They correspond to the rotation with a negative projection of angular velocity and to rotation with positive projection of angular velocity with various tangent of angle of an inclination of dependence.

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Dusty plasmas in non-uniform magnetic field

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The stability problem of striations is of paramount importance when studying dusty plasma in a magnetic field under a glow discharge, which is characterized by ionization and intense electron and ion flows in striations. The stratified mode of the discharge arises at emergence of heterogeneity in the channel of current: a narrowing or a turn of discharge tube, electric probe under high potential and other.

In the present report, the heterogeneity of the longitudinal field at a solenoid end face is applied to a formation of standing striations in magnetic field. In the found dust trap the volume dust structure which levitates in the area of strongly non-uniform magnetic field near end face of the superconducting solenoid is created.

The picture of the movement of the structure in strong magnetic field is experimentally registered; the mechanisms, first of all, a gradient drift of the ion components, leads the found structure to mechanical motion are discussed.

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Differential rotation of dusty plasma formed in striation of glow discharge in strong magnetic field

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The data of an experiment on a research of dust structures in standing striations of the glow discharge in strong magnetic field up to 10000 G are presented in this work. A task of the work was to localize an area of emergence of the mechanisms untwisting the dust structure inside the striations. The extended structures reaching the size up to 1 cm along an axis of the discharge and containing several hundreds of particles have been obtained. Polydisperse quartz particles were used, observations were made in neon under standard conditions for similar experiments. For a creation of magnetic field the superconducting magnet allowed to obtain the uniform vertical field in the area of placing of the dust trap was used. Angular velocity of rotation of horizontal sections of dust structure depending on their vertical coordinate at several values of magnetic field was measured. The linear dependence of angular velocity of horizontal sections of dust structure on vertical coordinate is found. Upper sections of structure have the larger value of angular velocity in comparison with lower ones. The inclination of straight lines on a graph of the dependence of angular velocity on a height within an error of measurements is almost identical for the chosen values of magnetic field. The estimated gradient of angular velocity is about 2 rad/s cm. The obtained results confirm a hypothesis of untwisting of dust structure by the rotating discharge gas owing to action of Ampere force on the eddy electron current. Geometrically this mechanism works in a tail part striations. In our experiment the top part of structure which rotates with a bigger angular velocity is located there. Work is supported by the Russian Science Foundation, grant No. 18-12-00009.

Influence of magnetic field on the dynamics of charged particles in restricted systems

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In this paper, we reported on the results of numerical and analytic study on a constant magnetic field and dynamic thermal motion of charged particles in an isotropic electrostatic trap. The simulation was carried out for cluster systems consisting of approximately up to one thousand particles with the Coulomb interaction in a wide range of their parameters.
Analytical relations for the spectral density of displacements of the center of mass of the studied systems are considered. These relations are verified by numerical simulation for clusters with different numbers of particles in a wide range of parameters of the analyzed systems. The features of the mass transfer and diffusion regimes of the motion of charged particles in restricted ensembles are studied in detail. The analysis of particle dynamics was performed depending on their number, temperature, and the magnitude of the magnetic and electric fields.
The results of this study can be used for restricted systems for any type of pair interactions and can be useful for developing new methods of diagnostics of physical characteristics of such systems and for analyzing the condition for the formation of various clusters, which are of interest for the plasma physics, polymer physics and colloidal systems, etc.
This study was supported in part by the Russian Foundation for Basic Research (project No. 18-38-20175) and was performed under the program of the Presidium of the Russian Academy of Sciences.

Comparison of megaampere channel temperature value measured by different methods at its maximal contraction in high density gas

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Comparison of discharge channel temperature in high density hydrogen with current amplitude of $\sim$ 1 MA at initial gas pressure of 5–7 MPa, determined by various methods, was done under stage of its maximal contraction. In the first case determination of the temperature value of 72–73 eV was made by intensity of soft x-ray radiation from the channel for experiments with current amplitude of 1.1–1.5 MA [1]. The estimation of the temperature on the basis of the data received by magnetic probe method and specified electric characteristics of the channel was of $\approx$ 140 eV for experiment with initial gas pressure of 5 MPa at current amplitude of 0.93 MA. The temperature determination by the last procedure had small accuracy caused by the limitation of the magnetic probe technique in determination of the channel contraction ratio [2] and some assumptions for nearelectrode voltage drops calculations by this way [3]. Apparently, the channel temperature in stage of maximal contraction is of $\sim$ 100 eV.

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On the structure features of current filaments in atmospheric discharge

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Recent studies of the structure of emerging breakdown channels in a strong nonuniform field at atmospheric pressure with temporal resolution show [1] that structures with a micron spatial scale and high electron density are formed at the very beginning of the breakdown development. At this point, a significant current flows through the discharge gap. There is a complex spatial character of the growth of microchannels: a change in the direction of growth, branching, closure, etc on a longitudinal scale comparable to the transverse size of the channels. With a relatively long lifetime of the formed microchannels, up to the main stage of the discharge, at the early stage of their formation, on a much smaller time scale, effects are possible that are related by the spatial arrangement of the individual microchannels. So, the closure of several nearly located microchannels with a length of several hundred microns can be considered as switching of several conductors, which are long lines in the picosecond time range.We discuss possible scenarios of "electrical" obtaining potentials higher than those applied in the nascent discharge due to the transformation of the applied voltage in the evolving structure of current microchannels. Such a local "voltage multiplication" can be one of the mechanisms for the occurrence of high-energy radiation (with quantum energy significantly higher than the applied voltage) in the initial phase of a high-voltage atmospheric discharge [2]. The work was supported by the Russian Foundation for Basic Research, grants No. 17-08-01690 and 19-02-00465.

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Recording and analysis of radio emissions in the initial phase of the spark atmospheric discharge

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The processes occurring in the initial phase of high-current pulsed atmospheric discharges, leading to the generation of various radiations have long been studied. Narrowband 2.4 GHz radio pulses is observed in [1]. In [2] radiation was observed with a ceramic patch antenna and a digital radio receiver tuned to a center frequency of 1.63 GHz and a bandwidth of 2 MHz.

In this work, we describe the antennas, modeled and calculated in the software package CST Microwave Studio for the needs of the experiment. A characteristic feature of the new antennas has the best coordination and amplification of signals at frequencies in the GHz range. The antennas were used to record radio emissions from spark discharges at three different experimental facilities, which allow to obtain spark discharges of meter, centimeter and millimeter length, and differ in the time of rise of the voltage pulse and the field distribution in the interelectrode space. The report presents the spectra of the measured radio signals and describes the observed dependence of the radiation characteristics on the change in the discharge parameters.

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Features of laser interferometry of plasma objects appearing within spark channel formation in a nanosecond air discharge

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Approaches to processing the results obtained using laser interferometry and photographing by Schlieren of highly ionized near-cathode plasma arising due to a strong explosion at the moment of breakdown of the gap are presented. Within the discharge formation in air the near-cathode plasma appears as the fringes with a negative curvature and closed circular fringes in the interferograms, which require a special procedure for processing. The specialty of the procedure is the small size and complex structure (e.g., geometry) of the object. To process the interferograms and reconstruct the electron density distribution of the studied plasma, the smooth perturbation method, described in [1], is used to solve the Helmholtz equation. To clarify the object parameters, by varying its geometry and density distributions, we additionally simulate its model interferograms and schlirien images. We demonstrate that the spark channel originating from the cathode can be treated as a solid cylinder with the maximum electron density at its axis with a plasma sphere having the minimum electron density inside and the maximum density on its boundary connecting the cylinder with the cathode.

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Filamentary instability and its role in the spark discharge formation in an atmospheric discharge

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Formation of a millimeter-sized spark discharge in standard temperature and pressure air was studied on a nanosecond time scale using multi-frame laser probing with an exposure time of 70 ps and spatial resolution as high as 3–4 μm. We found that the growing spark channel develops in the form of multiple ($N \gtrsim 10$) filaments that constitute plasma channels with micron-sized ($\sim$ 10–50 μm) diameters, the electron density of $n_e \sim 10^{19}$–10^{20} cm^{-3}, and characteristic evolution time less than 1 ns. It is demonstrated that the first filaments are formed at the top of the developing homogenous spark channel. Further, the growing filaments are split themselves, and their number is increased up to several tens. Our findings indicate that the spark channel filamentation is one of the important mechanisms that govern the current capacity and the resistivity of the discharge gap after the breakdown. Additionally, the spark channel filamentation plays a key role in the discharge formation at high pressures on the nanosecond time scale. The obtained data on the evolving filaments can provide a groundbreaking basis for creating a comprehensive model for calculating the spark channel resistance for purposes of high-current electronics. We also suppose that the possible development of the filamentary structure can have a significant impact on the formation of leaders or long sparks as well as the origination of natural lightning.

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Cathode explosion gives rise to the spark channel development during the discharge formation in air

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Formation of a millimeter-sized spark discharge in standard temperature and pressure air was studied on a nanosecond time scale using multi-frame laser probing with an exposure time of 70 ps and spatial resolution as high as 3–4 μm. We found that the instant of the breakdown is associated with fast ($\ll 1$ ns) formation of a micron-sized (~ 10 μm) cathode spot [1]. The spot appears as a highly ionized near-cathode plasma with an electron density of $n_e \approx 10^{19}$ cm^{-3}. Further, this plasma transforms into a highly ionized spark channel with an electron density of $n_e \sim 10^{19}$–10^{20} cm^{-3}. The formation of the near-cathode plasma is similar to the violent explosion of a small part of the cathode surface that is accompanied by ejection of the cathode material (dense plasma with $n_e > 10^{20}$ cm^{-3}). Our findings indicate that the dynamics of the highly ionized near-cathode plasma governs the current capacity of the discharge gap as well as the initial current rise rate.

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The origin of plasma jets generated in Z-pinch discharges

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Z-pinch discharges are well known by generation of electron beams, neutrons, hard and soft x-ray emission, etc. One of the most interesting feature of Z-pinches is plasma jets spreading along the discharge axis. Despite of this phenomena was many times registered in experiments there is no concrete information about its nature. One of the main hypothesis assumes that plasma jets have cumulative origin similar to the one which takes place in cumulative shells. The current sheath in Z-pinch has conical shape when comes to discharge axis, and it looks very similar to conical shells mechanically fabricated in cumulative shells. So it was really a temptation to apply the theory of hollow charge explosions which considered the generation of cumulative jets, to formation of plasma jets in Z-pinches.
In this paper, we present the results of two-dimensional magnetohydrodynamics (MHD) numerical modeling of plasma jets generated in Z-pinches. Z-pinch discharge is studied starting from the very beginning (breakdown near isolator) up to the end (plasma cooling). The development of current sheath, its conical structure and formation of plasma jets are visibly predicted by the modeling. MHD study has shown that plasma jets are generated when conical current sheath is already disappeared. Plasma is compressed in radial direction by magnetic field pressure with further expected outflow in axial direction. That is why the origin of plasma jets in Z-pinches is not a cumulative effect, but magnetic field pressure. MHD modeling is also carried out for q-pinch systems where generation of plasma jets was not found. The corresponding analysis are presented.

Study of plasma jets in plasma focus using the snow-plough model

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A collapse of conical shells in the projectiles was studied by theory of hollow charge explosions. In plasma experiments, the purely hydrodynamic effect, which takes place in solid explosives, is replaced with the magnetohydrodynamic effect, which accelerates plasma up to higher velocities. Current sheath (CS) in plasma focus discharges (PFD) moves along the discharge axis and the speed of CS achieves (3–5)$\times 10^7$ cm/s. At the compression stage dense and hot plasma is created, plasma jets (PJ) are generated along the discharge axis. The important applications of the PJ are acceleration of macro particles, investigation of plasma–surface interaction, modification of constructional materials with the aim to impart new properties, laboratory modeling of astrophysical phenomena, etc. Numerical modeling of PJ which predicts optimal generation conditions might help to understand PJ nature and to decrease the cost of corresponding experiments. In this paper, the investigation of PJ in PF-4 machine is made by the snow-plough model, which assumes that discharge current is concentrated inside CS which moves due to ponderomotive force. Discharge chamber is divided by CS into two areas, the one (behind CS) is filled with working gas, the other one (in front of CS) is filled by magnetic field which is determined by current, flowing through Z-pinch. Numerical study has shown that optimized PF-4 machine generates plasma jets with axial speed 5×10^7 cm/s, few times exceeding the speed of thermal plasma expansion. It means that long distance transportation of plasma jets can be effectively achieved. Results of calculations are in good agreement with experiment carried out by shearing interferometry.

Thrust of synthetic jet and power characteristics of plasma actuators at reduced pressure

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Symmetric actuators creating a dielectric barrier discharge (DBD) can be used to control the lift force of the wing [1]. Under the action of strong electric field, a surrounding air ionizes and accelerates. This leads to the formation of the synthetic jet, directed perpendicular to the surface of the wing in a given area [2]. For a greater effect of the impact of synthetic jet on the flow the thrust must be greater with less energy coupling. At atmospheric pressure there is a lot of information about the dependencies of thrust of the synthetic jets vs. a number of parameters. In this work, the dependence of linear thrust and specific thrust to power of synthetic jets produced by symmetric actuator with various configurations vs. air pressure corresponding to flight altitudes up to 20 km was investigated. At certain pressures, there are maxima in the dependencies. Maximal linear thrust indicates that the jet produces the maximal control force. The maximal ratio of thrust to power indicates that the actuator most efficiently converts electrical energy into kinetic energy of the jet. The existence of maxima is explained by the theory based on the resonance mode of operation of the system: power supply-actuator-DBD. This work was supported by the Presidium of the Russian Academy of Sciences, program No. I.56.

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On the efficiency of dielectric barrier discharge at various pressures

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For controlling the flow around the wings of an airplane, a dielectric barrier discharge (DBD) created by a plasma drive can be used [1]. The flight speed should be no more than 25 m/s; the Reynolds number Re $\approx 10^4$. Such conditions are achievable when flying unmanned aerial vehicles at an altitude of about 20 km. As the height increases, the pressure and temperature of the ambient air changes. Therefore the characteristics and properties of the DBD are also changing. Most of the existing works have been carried out at atmospheric pressure [2, 3].

In this paper, we investigated the electrical characteristics of DBD under reduced pressure. Methods have been developed for measuring the capacity of the actuator, the inductance of the "power supply–actuator–DBD" system and the electrical capacitance of the discharge. The dependences of the resonant frequency and system dissipation coefficients, discharge efficiency are determined. The results show that with a decrease in pressure, the discharge efficiency increases significantly.

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Generation of the sliding discharge on the wedge in a supersonic flow

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Sliding discharge was generated in a supersonic atmospheric-vacuum wind tunnel with a flow Max number M = 2, Reynolds number of about 10^6, and static pressure in the flow $p = 0.15$–0.18 atm. The discharge region was located perpendicular to the flow lines. The discharge length was 5 cm. Discharge initiation system was consisted of the ballast resistance R, whose value was determined by the maximal output current of the high voltage source for the given voltage, and a set of high voltage condensers. The condenser charging time is on the order of RC, and this quantity determines the frequency of discharge initiation in the flow. The condensers voltage was 5 kV. By changing the capacitance C, it is possible to change both the energy of a single pulse and the frequency of pulse repetition.

The force arising from the interaction of the discharge with the flow was measured using a strain gauge. The schlieren visualization of the flow was also performed. It was found that the impact of the discharge is not limited by the appearance of a weak shock wave, and also significantly changes the properties of the flow around the wedge due to pulse heat generation. With a single initiation of a discharge with an energy of 125 J without flow, no significant force was recorded, both at atmospheric and at reduced pressures. In the flow, a single sliding discharge of the same parameters created a force of about 1.5 N. As the discharge energy increases, the force from its impact on the wedge also increases. Force produced by the sliding discharge in the supersonic flow is several times greater than in the static air regardless of its pressure in the range from 0.15 to 1 atm.

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Critical runaway electron avalanche

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The x-ray and γ-ray flares observed in the thunderstorm atmosphere of the earth are usually associated with the generation of runaway electrons (RE) in electric atmospheric fields. It is assumed that in avalanche discharges, which are observed in a thunderstorm atmosphere, the main role is played by avalanche of RE, initiated by cosmic rays. In this paper, using the three-dimensional numerical calculations, the development regularities are investigated and the parameters of the critical avalanches are determined. It is shown that in air under conditions characteristic of thunderstorm atmospheric discharges, the number of electrons in the critical avalanche of RE can reach values of the order of 10^{18} particles [1]. The work was supported by the Russian Academy of Sciences.

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To the presence of runaway electrons and electron avalanche formation in nuclear induced helium plasmas

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In this work, the Boltzmann kinetic equation for plasma generated by volume source of ionization is developed and solved for special cases, like presence of external electric field, strong enough to cause Townsend ionization. The ways of possible existing of highly energetic electrons accelerated by strong electric field energy also thoroughly discussed. Statistical approach based on the Monte Carlo technique including definition of self-consistent electric field formed by boundary conditions and nuclear induced plasma internal properties coupled with direct Boltzmann formalism also was developed and discussed. Thus the outbreak or the time explosion of the energy distributions of all fast particle including primary and secondary electrons are calculated in the programming complex as a function of time from 10 ps to 10 ns and for different neutron flux pulses and neutrons homogeneous spatial distribution. Non-linear problems such as an electron–ion recombination and successive generation of secondary electrons and electron queues are solved by Monte Carlo technique and comprehensively described. Detailed calculations show that so called runaway electrons are not appearing in nuclear induced plasma and whatever strong external electric field applied, there is no way to supply them relativistic energy and create so called runaway electrons. The appearance of electrons with an energy around MeV is possible when electrons (beta electrons) are born within nucleus due to internuclear transformations of up and down quarks affected by neutrinos oscillations.

Comparative analysis of ways of arc initiation in alternating current plasma torch with rail electrodes

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One of the main factors determining the high reliability and usability of powerful plasma torches in the composition of electro-physical installations [1] for various purposes is the question of arc initiation in the electric arc chamber of the plasma torch. The traditional solution is a plasma injector using a high-voltage alternating current plasma torch. Its power is about 10 kW, the flow rate of plasma-forming working gas is up to 5 g/s. When the injector is operating in the zone of minimum distance between the main electrodes of the plasma torch, a plasma flow is established with a sufficient concentration of electrons to ignite the main arcs. The paper describes the performed experimental studies on the efficiency of the pre-ionization modes of the interelectrode gap in order to ensure stable ignition of the main arc, trouble proof and reliable operation of the plasma torch with rail electrodes. A comparison of characteristics life, reliability and cost solutions for the replacement of the existing pre-ionizer—a high-voltage single-phase alternating current plasma torch with a power source based on a high-voltage transformer and current-limiting chokes is presented.

[1] Safronov A A, Vasilieva O B, Dudnik Y D, Kuznetsov V E, Shiryaev V N, Subbotin D I and Pavlov A V 2017 *J. Phys.: Conf. Ser.* **825** 012013

Radiation energy losses in a single chamber three phase plasma torch with rod electrodes

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As a rule three phase single chamber plasma torches have a comparatively small length so that a rather high efficiency is provided [1]. Unlike plasma torches with the linear scheme, electrodes, where the arc is ignited, are located in one level, so-called the electrode block. The main losses of energy are radiant losses as long as plasma torch length is less than length of the initial section of the gas flow supplied in a plasma torch, on which the thermal layer of an arc does not interact with its turbulent layer [2]. At the same time a conic part of the chamber apart from radiant streams also perceives energy streams due to the convection, i.e. a conic part is subjected to the difficult heat exchange consisting mainly of radiant and convective heat exchange. The purpose of work consists in determination the share of radiant losses in the general system of heat losses and also the relative value of emitting power of a three phase single chamber plasma torch. Experiments were carried out on a nitric alternating current plasma torch with tungsten electrodes at pressure 0.1–5.7 MPa, nitrogen flow 0.03–0.08 kg/s. The maximum current is short circuit current 330 A. Energy losses in a wall of the electrode block and a conic part of the camera were determined separately by calorimetric method by the cooling water. The sum of these losses made the general losses by which plasma torch efficiency was determined.

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[2] Zhukov M F, Koroteev A S and Uryukov B A 1975 *Prikladnaya Dinamika Termicheskoj Plazmy* (Novosibirsk: Nauka)

Energy balance in highly ionized nonequilibrium helium plasma

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In previous works, studies were performed on highly ionized helium arc plasma at atmospheric pressure under nonequilibrium conditions in narrow plasma channel with diameter of 2 mm. It was shown [1] that radial inhomogenity is one of the reasons for ionization nonequilibrium taking place at the discharge axis despite high values of electron concentration ($n_e \sim 10^{17}$ cm^{-3}), and electron temperature (T_e = 3.2–4.7 eV) determination methods for nonequilibrium conditions was developed [2]. This work is on energy balance of such plasmas, which was not studied in the previous publications. Electron energy loss consists of two factors: elastic (W_{el}) and inelastic (W_{in}) interactions with heavy components of plasma. The value of W_{el} takes place due to nonisothermic nature of this kind of plasma ($T_a < T_e$) and consist of atomic and ionic scattering losses. However, atomic component contribution is low and can be omitted. The value of W_{in} is the sum of the energy effects of a large number of bound–bound and bound–unbound electronic transitions which are mostly mutually balanced and do not contribute to the energy balance. Inelastic transitions, which are not mutually balanced, arise only due to nonequilibrium processes of interaction between excited and charged particles. In our case, these are mainly ambipolar diffusion processes, when charged particles leave the plasma volume and are transferred to the plasma torch channel walls.

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[1] Kavyrshin D I, Chinnov V F, Sargsyan M A, Korshunov O V, Ageev A G and Efimov A V 2016 *J. Phys.: Conf. Ser.* **774** 012200

[2] Kavyrshin D I, Chinnov V F, Korshunov O V and Ageev A G 2016 *J. Phys.: Conf. Ser.* **774** 012199

Plasma jet velocity measurement by stereoscopy visualizing the motion of optical inhomogeneities

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Low-temperature plasma jet is a widespread object to research, and plasma flow rate is one of its most important characteristics. Authors have recently proposed and tested the method for determining of the submerged plasma jet velocity ($V \leqslant 1000$ m/s) using a high-speed camera based on measuring and analyzing the movement of optical inhomogeneities (OI) that are specially injected into plasma stream [1]. As a source of OI an extent thin graphite rod (much thinner than the diameter of the jet) was used, it was injected into the plasma flow in a transverse direction with an electromagnetic drive. OI are micron size products of evaporation and ablation of the rod material and interaction products of plasma and rod material, so they are picked up by plasma stream and quickly ($\tau \leqslant 3$ μs) acquire its speed. In this paper, the method has been developed that uses two high-speed cameras synchronized by frames per second, one of which is a colored camera and is at some angle to the other (i.e., stereoscopy method). The authors showed that the use of such a schematic makes it possible to clarify the location of any OI in the plasma jet and determine both components of its velocity. It was found that the color image of the plasma flows spread region opens up the possibility of determining the velocity of the OI and of the jet itself at the same time due to the color differentiation of their images in the frame.

The work is supported by the Russian Foundation for Basic Research (project No. 17–08–00816).

[1] Chinnov V 2017 *Int. Conf. on Phenomena in Ionized Gases XXXIII ICPIG* 238

Stochastic nanostructure and fuzz-like structure formation on the material surface under powerful plasma load in the plasma linear multicusp device

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The plasma linear multicusp (PLM) device was constructed to test materials by powerful plasma loads. The facility is a linear magnetic trap with a 8-pole multicusp magnetic plasma confinement. In the PLM, the electron temperature of the hot and cold fractions are of 50 and 10 eV respectively, the electron density—2×10^{18} m^{-3}, the stationary plasma confinement is up to 200 min and more, which is an advantage for testing materials of the divertor and first wall of a fusion reactor. Tungsten, molybdenum, graphite, iron were irradiated with stationary helium plasma in the PLM with the thermal load of more than 1 MW/m^2. The temperature of the tested plates reached 1000 °C and more. A stochastic nanostructured surface and fuzz-like structure with fibers of less than 50 nm in a diameter were observed on the irradiated plates. This work was supported by the grant of the Russian National Science Foundation 17-19-01469, the production of the automated research system at the PLM was supported by the Russian-Federation Megagrant No. 14.Z50.31.0042.

On the dynamics of high-density cathode-spot plasma in a magnetic field

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The plasma dynamics is determined by the explosion-emission cells of the cathode spot of the vacuum arc in a magnetic field. It was shown that the expansion of plasma (high density) in a transverse magnetic field can cause asymmetry in the distribution of plasma density at the boundary of the cathode spot. Asymmetry, in turn, increases the probability of ignition of new explosion-emission cells in the region of a stronger magnetic field in the "anti-ampere" direction $\mathbf{B} \times \mathbf{I}$. The disturbed plasma density distribution estimated in the molecularhydrodynamics approximation is presented. In addition, the velocity of the "retrograde" spot motion (ignition of new explosive-emission cells) in the stronger field region is estimated as a function of the external magnetic field strength. The velocity estimates [a few to tens of m/(s T)] are shown to agree with experimental data.

The work was supported in part by the Russian Foundation for Basic Research, grant No. 19-08-01249.

Implosion of composite wire arrays powered by microsecond current pulses with amplitude up to 2 MA

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This paper presents the results of experiments concerned the implosion of composite multi-wire cylindrical arrays (wires of different diameters) powered by microsecond current pulses with the amplitude up to 2 MA. The goal of the performed experimental works lies in generation of high-power time shaped soft x-ray pulses to study spectral radiation runs in a substance at high-energy densities. Numerical simulation of the dynamical Z-pinch was carried out in the frameworks of the magneto-hydrodynamic code FLUX-3D. Preliminary experimental mass scaling of the imploding single cylindrical arrays was carried out for benchmark of the calculated model. The arrays consisted of 45 tungsten wires of the diameters from 4 to 15 μm and height of 30 mm. The wires were evenly located on the cylindrical surface of 3 cm radius. Features of the imploding arrays composed of the wires of different diameters are analyzed. Different regimes of the current distribution on subsystems of the wires of different diameters are considered. Shaping of soft x-ray pulse was obtained: we recorded the pedestal before the main radiation pulse. Its length is four times more than the radiation pulse and about 20% of its amplitude. It was revealed that application of the composite arrays decreases efficiency of the soft x-ray pulse generation. The reasons are: unsimultaneity of the plasma ablation end in different wires subsystems and appearance of large azimuth heterogeneity that negatively affects the tightness of final compression of the plasma. Results of the composite arrays numerical simulation match the x-ray streak camera data and bolometer measurements.

Verification experimental studies of pulsed plasma accelerators

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Explosive-magnetic generators (EMG), in contrast to the capacitive storage (CS), as a rule, have a growing power. The effective operation of pulsed plasma loads, such as pulsed plasma accelerators (PPA), plasma focus, plasma breakers, etc, can be provided at realization of the mentioned advantage of EMG as a power source. The technique of laboratory verification experiments with PPA powered by CS, which precedes the explosive experiment with a power source from EMG, is presented in the report. In the experiments, the electrical parameters CS and PPA were recorded. The dependencies of the load operation modes on the start parameters, including the dynamics of the inductance and the position of the current shell inside the PPA, are determined by the analysis of the data. The method allows reducing the number of expensive explosive experiments and supplements the database of nonlinear dependencies of the load parameters under various amplitudes of the current pulse. This work is important for mathematical modeling of power supply and plasma load matching problems. These experimental studies together with the calculated model of operation of the EMG on a non-linear load, allow preliminary coordination such loads with EMG. Thus, the productivity of experiments with EMG increases greatly. The developed technique can be adapted to a wide class of nonlinear loads.

Plasma method of zinc oxide obtain

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Zinc oxide is the most important substance in the chemical industry. The number of catalysts and sorbents based on it is very large. For its more effective use, the produced zinc oxide must be sufficiently strongly dispersed. Zinc oxide is obtained by oxidation of gaseous metallic zinc with oxygen, thermal decomposition of its salts, hydrothermal synthesis and calcination of zinc sulfide. One of the methods for obtaining fine powder of zinc oxide is the plasma method. Most often, oxide powder is fed into the thermal plasma stream. The report deals with a modified the plasma method. An aqueous solution of zinc nitrate is fed into the stream of air plasma. The facility consists of the ac plasma torch, a reaction chamber, and a solution supply device. Due to the dilution of the precursor, sufficiently small solid particles are formed. At the same time, as the temperature rises, zinc nitrate decomposes to form zinc oxide, and water evaporates. During the experiments, the power of the plasma torch was up to 6 kW, and the concentration of the solution was 0.05 and 0.1 mol/l. The produced zinc oxide was deposited on the water-cooled surface. The composition and properties of the powder were studied on an x-ray diffractometer, an ir spectrometer and a scanning microscope. Indeed, the relatively strong dissolution of the solution resulted to the production of nanoscale particles. However, the use of water is very energy intensive, so it is advisable to use a substance as a solvent with lower values of heat capacity and heat of evaporation.

Propane reforming by carbon dioxide thermal plasma

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Hydrogen is the most popular product in chemical technology. It is produced by steam reforming of natural gas and gasification of solid fuels. However, it is known that associated petroleum gas can also be used as a feedstock for hydrogen production. Currently, the associated gas in large oil fields is not used (it is burned), which causes carbon dioxide emissions to the environment. The main components of the associated gas are methane, propane and ethane. The report deals with carbon dioxide plasma propane reforming. It is known that the energy consumption for carbon dioxide reforming is greater than the cost of steam reforming. However, carbon dioxide was chosen to reduce the harmful effects on the environment. The evaluation was performed under stoichiometric conditions (thermodynamic equilibrium). It is established that at a temperature of more than 1140 K there are no solid substances (soot) in the reaction products. The minimum specific flow rate of carbon dioxide is 0.33 kg/kg propane. The composition of the product gas is as follows: CO—59.8 vol %, H_2—38.6 vol %, CO_2—0.9 vol %, H_2O—0.7 vol %. Obtained results were compared with experimental data. The experiment was carried out on a facility consisting of a three-phase ac plasma torch and 70-L lined reactor. The plasma torch is three cylindrical arc channels with two gas input zones: the electrode zone (for carbon dioxide) and the arc zone (for propane).

Study of ozone production in a dielectric barrier discharge in oxygen-containing mixtures for plasma assisted combustion

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The paper presents the results of measurements of ozone number densities [O_3] in a "diffuse" barrier discharge at an atmospheric pressure in air, oxygen, and in a mixture of oxygen and methane. For various experimental configurations, the dependences of [O_3] on discharge power are obtained. Experimental data and the results of numerical simulations were compared. These results are necessary for the development of a numerical model of a barrier discharge, in particular, for plasma assisted combustion.

Surface barrier discharge pre-sowing treatment of winter wheat seeds in the three-electrode arrangement with dc bias

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In this paper, the experimental results of reaction of morphological indicators of seedlings of high quality winter wheat seeds treated by plasma byproducts in three-electrode system of the surface dielectric barrier discharge with direct current (dc) bias on the third electrode in humid air of atmospheric pressure at different polarity of the bias voltage are shown. The treatment was carried out for 15 min in the strip electrode system (eight 1 mm width strips with 4 mm distance between them, a sinusoidal voltage of 2.7 kV with a frequency 23 kHz) made on a alumina ceramic barrier (1 mm thickness) with the additional third electrode which is a stainless steel grid distant 10 mm from the surface of the dielectric barrier. A dc bias of 8 kV of positive or negative polarity was applied to the third electrode. Seeds were located on the surface of the third electrode. The treatment was also carried out with vibration of the system (the imitation of seeds movement along the third electrode). It is shown that the efficiency of treatment depends on the month of carrying it out. It was succeeded to get a reliable stimulation with weak control. With strong control (potential sowing months) it was not obtained. The imposing of dc bias in any considered case is less efficient than the affection of plasma products without bias.
The work was supported by the Russian Science Foundation (project No. 18-76-10019).

Study of a discharge with a liquid cathode with organic impurities

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The dc discharge between the electrode and the surface of the liquid is a promising object of study, both in terms of the applicability of such discharges in plasma-chemical technologies, and in terms of lack of knowledge of the processes occurring in such a discharge [1]. The video data was compared with another study of the plasma in this discharge that was performed using the methods of emission spectroscopy. Electrical parameters of the discharge were also measured. Sodium hydroxide solution in deionized water with a concentration of 60 mg/l (specific electrical conductivity 330 μS/cm) was used as a liquid cathode. The discharge occurred at atmospheric pressure in the air. The study was conducted in the range of currents 25–100 mA. The effect of organic impurities in the solution (alcohols, phenols) on the current-voltage characteristics and emission spectra of the discharge plasma was investigated. Deciphering the emission spectra of the discharge with a liquid cathode showed the presence of OH-radical emission bands and molecular nitrogen N_2, as well as lines of atomic hydrogen H and oxygen O. The dependence of the distributions of intensities of individual lines and bands on the distance to the surface of the liquid was investigated. It is shown that the distribution of the intensity of the luminescence of the OH-radical band substantially depends on the discharge current and impurities of organic compounds in the solution.

This work was partially supported by the Russian Foundation for Basic Research, grant No. 19-08-00592.

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Thermocouple and electric probe measurements in a cold microwave atmospheric-pressure plasma jet

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At the present time, the possibility of using atmospheric-pressure plasma jets is actively investigated in applications for plasma-chemical treatment of surfaces of various materials in such industries as practical medicine, microbiology, agriculture and food industry. The interest is due to the fact that in such jets so-called "streaming-afterglow" plasma is generated and excited plasma particles and radicals with high reactivity are produced. At that, the temperature of the gas flow can be reduced to almost room temperature, which does not have a destructive effect on a material during processing. It should be noted that for many plasma technologies, such as plasma cleaning, surface activation, deposition and etching, an important characteristic of a plasma source device is the area of the surface to be treated. The size of the outlets of most existing plasmatron burners (torches) is less than 1 cm in diameter. For a wide-area surface treatment, various tricks are used such as surface scanning or using of array of several burners. We present the prototype of the multi-purpose microwave plasmatron, which has a portable discharge torch with an outlet of 2.5 cm in diameter. Cold plasma jet outside the torch is operated by electrode 2.45 GHz discharge in the torch chamber. Oscillograms and floating potential dependences on distance from the torch outlet were measured for the planar electric probe. Gas temperature spatial distribution into the plasma jet was obtained by means of thermocouple method.

The work is supported by the Russian Foundation for Basic Research (project No. 19-08-00844).

Theoretical research of optimal configurations of rf ion thruster

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Mathematical models of plasma in the discharge chamber of a radio-frequency (rf) ion thruster are presented. The numerical-analytical zero-dimensional model of the thruster includes the joint solution of the equations of the balance, model of conservation of particles and energy, and the equations of the transformer model describing the interaction of the rf generator and the plasma load [1]. Using With this model, the search range of thruster modes and the integral plasma parameters are determined.
A two-dimensional axisymmetric model of a gas-discharge chamber, based on the kinetic approach of describing the discharge plasma, is also considered. The kinetic approach is implemented using the particles-in-cell method in the program code KARAT [2]. An analysis has been conducted of the complex influence of the gas-discharge chamber and rf antenna configuration on the distribution of magnetic fields. Ways of increasing ionization efficiency has been identified with regards to the percentage of the rf power coupled to plasma. An optimal discharge chamber geometry has been introduced, as well as the rf antenna operating mode. Recommendations have been formulated as to how such devices are to be calculated.

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[2] Tarakanov V P 2017 *EPJ Web Conf.* **149** 04024

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