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The book consists of abstracts of plenary lectures, oral reports and posters presented at the XXXVI International Conference on Interaction of Intense Energy Fluxes with Matter (1–6 March 2021, Elbrus, Kabardino-Balkaria, Russia). This conference is devoted to the 75th anniversary of birth of Academician Vladimir Evgenyevich Fortov (23 January 1946 – 29 November 2020). The conference topics are as follows: interaction of intense laser, x-ray and microwave radiation, powerful particle beams with matter; experimental techniques of generation and diagnostics of extreme states of matter; shock waves, detonation and combustion physics; equations of state and constitutive equations for matter under extreme conditions at high pressures and temperatures; methods of mathematical modeling in physics of extreme states of matter; high-energy astrophysics; physics of low-temperature and non-ideal plasma; physical issues of power engineering and technology aspects.

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The editorial board with deep regret announces the death of friends and colleagues: Professor Andrey Nikonovich Starostin (25 February 1940 – 16 April 2020); Professor Igor Korneliyevich Krasyuk (7 March 1942 – 26 May 2020); Professor Boris Alekseyevich Demidov (03 April 1935 – 3 June 2020); Professor Valentina Feognievna Degtyareva (12 March 1940 – 12 September 2020); Professor Alexander Iosifovich Funtikov (1 December 1932 – 15 September 2020); Corresponding Member of the Russian Academy of Sciences, Professor Nikolay Nikolayevich Kalitkin (16 August 1935 – 7 January 2021); Corresponding Member of the Russian Academy of Sciences, Professor Gennady Isaakovich Kanel (30 June 1944 – 31 January 2021); Professor Andrey Andreyevich Deribas (13 June 1931 – 25 February 2021). All of them were active participants in this series of conferences.

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1. Power Interaction with Matter

Laser action: Structuring, peening and microfabrication of laminates

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Knowledge of the physics of the effect of laser radiation on matter is important for many modern technologies.
Structuring: In the experiment, two identical fs laser pulses were used. They are separated in time by 200 μs. The first pulse creates a bubble. The bubble is filled with products of high temperature chemical decomposition of liquid. The microbubble has submicron or micron sizes. The second pulse undergoes diffraction scattering on a bubble. Thanks to diffraction, a bright ring (instead of Gaussian distribution) of illumination appears and is imprinted on the target.
Nanolaminates: The laser impact on laminates is fundamentally different from the impact on a homogeneous target. Echoes of reflections from contacts appear. During thermomechanical ablation of laminates, spalls within the layers alternate with spalls along the contacts between the layers.
Strengthening: We consider formation and propagation of laser shock waves (SW) generated by an ultrashort laser pulse. Our approach takes into account polymorphic phase transitions in the solid phase and geometric effects—the transition from a quasi-plane propagation regime to a three-dimensional (3D) SW. The fact is that the laser heating depth is small compared to the radius of the laser spot. Then the transition to the 3D regime occurs when the path traveled by the wave becomes of the order of the spot radius.

Picosecond laser action on iron films: Elastic, plastic and polymorphic transformations

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The results of experimental, theoretical and numerical study of laser shock waves (SW) initiated by a picosecond (ps) pulse in iron are described. Picosecond impacts correspond to very high rates of deformation, unattainable by traditional means. Research is interesting for a number of reasons. It is important to understand how the rate of deformation affects elastic-plastic and polymorphic transformations. In particular, the study of this problem is necessary for the development of a consistent theory of ps laser hardening of metals, which is now making its first steps; although this kind of hardening approach (laser forging) is already widely used in practice. We performed a series of experiments. Modern developments in the field of SW generation and, most importantly, their experimental diagnostics are applied. Methods of theoretical interpretation of diagnostic data are developed. These methods are used for the first time in the class of ps effects. The fact is that the diagnostics of experiments only presents us with the kinematics of what is happening. Measurements of mechanical stresses (say, by means of manganin sensors) do not exist in ps experiments. Meanwhile, without data on stresses, the kinetics of polymorphic transformation remains unclear. Experiments are supported by hydrodynamic and molecular dynamics numerical simulations.

Atomistic simulations of nanoparticle generation by short pulse laser ablation of AgCu bilayers in liquid

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The ability of short pulse laser ablation in liquids (PLAL) to produce colloidal solutions of chemically clean nanoparticles has been employed in a broad range of practical applications. Large-scale atomistic simulations have yielded important insights into the fundamental mechanisms of PLAL [1,2] and provided a plausible explanation of the origin of the experimentally observed broad or bimodal nanoparticle size distributions [3]. In the computational effort reported in this presentation, we extend the atomistic simulations to investigation of the nanoparticle formation mechanisms in PLAL of Ag/Cu and Cu/Ag bilayer thin films. The nanoparticle compositions observed in the simulations exhibit an enhanced abundance of Ag-rich and Cu-rich nanoparticles and a strongly depressed population of well-mixed alloy nanoparticles. The computational predictions are verified in experiments performed at the University of Duisburg-Essen and Kiel University, Germany [4]. The surprising observation that the nanoscale spatial separation of the two components in the bilayer films manifests itself in the sharp departure from the complete quantitative mixing in the colloidal nanoparticles is explained by the complex dynamic interaction between the ablation plume and liquid environment revealed in the simulations.

[1] Shih C Y, Shugaev M V, Wu C and Zhigilei L V 2017 *J. Phys. Chem. C* **121** 16549–16567

[2] Shih C Y, Shugaev M V, Wu C and Zhigilei L V 2020 *Phys. Chem. Chem. Phys.* **22** 7077–7099

[3] Shih C Y *et al* 2018 *Nanoscale* **10** 6900–6910

[4] Shih C Y *et al* 2021 *J. Phys. Chem. C* in press, doi:10.1021/acs.jpcc.0c09970

Heating effects of high power THz pulses on water

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Exposure of cells or biological tissues to high-power pulses of THz radiation leads to changes in a variety of intracellular processes. However, the role of heating effects due to strong absorption of THz radiation by water molecules still stays unclear. In this study, we performed numerical modelling in order to estimate the thermal impact on water of a single THz pulse as well as a series of THz pulses. A finite-element model that provides numerical solutions for the heat conduction equation is employed to compute the temperature increase. A simple expression for temperature estimation in the center of the spot of THz radiation is presented for given frequency and fluence of the THz pulse. It has been demonstrated that thermal effect is determined by either the average power of radiation or by the fluence of a single THz pulse depending on pulse repetition rate. In order to estimate the thermal effect of THz radiation on living cells experiments on human dermal fibroblasts exposure to THz pulses (with an energy of 15 μJ and repetition rate of 100 Hz) have been performed. Analysis of heat shock proteins expression has demonstrated no statistically significant difference between experimental group after 3 h of irradiation and control group.

X-ray and THz generation from metal foil irradiated by laser pulses

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Powerful terahertz (THz) pulses can be used to excite non stationary states of matter via phonons, excitons, etc. We experimentally compare several methods to get efficient THz with femtosecond 800-nm laser pulses driver, the generation in metal case has an advantage (over nonlinear crystals or plasma) of efficiency increase with TW laser power. While much of cutting-edge research in relativistic electrodynamics is currently focused on THz generation from metal foils driven by relativistic laser pulses, here, we show that some yet-to-be-solved problems in laser–matter interactions can be addressed by studying THz emission from metal foils at lower, nonrelativistic levels of laser intensities. We observed the efficiency 10^{-5} of THz generation, that is higher than predicted by known theories for the intensity of 10^{16} W/cm^2. X-ray radiation from the same foil is analyzed. Characteristic K_α line is sufficient for x-ray fs diagnostics of nonstationary states of matter, providing 10^8 photons/sr/pulse. An important issue is to refocus x-ray radiation on the sample for (THz) pump-probe study with almost parallel and narrow beam. For that purpose we develop a special polycapillary lens. This work is supported by the Russian Foundation for Basic Research (grants No. 18-02-40032, 20-21-00140).

Fragmentation of a metal droplet irradiated by a polarized ultrashort laser pulse

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In this work, we present experimental and numerical study of a jet effusion from a metal droplet irradiated by a polarized ultrashort laser pulse. We demonstrated formation of cross-like structures as a result of droplet fragmentation, which are well correlated with polarization vector of the laser pulse. Our experiments show that rotation of polarization vector causes rotation of the structures in the same direction. Experimental results are interpreted using molecular dynamic simulations. Performed simulations show that the specific formation of jets, which is observed in experiments, is determined by the absorption asymmetry of a linearly polarized laser pulse. It is shown that asymmetric heating induces an inverse flow on the frontal and rear surfaces of the droplet, which promotes the formation of cross-like structures.

Laser-plasma assisted ablation of SiC

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Owing to its unique physical properties, silicon carbide (SiC) is a promising material for applications in power electronics, MEMS, nanophotonics and nanoelectronics [1]. One of the effective techniques of SiC processing is laser ablation [2]. Strongly depending on parameters of laser irradiation, the thikness of the removed layer at laser ablation achieves ~ 1 μm per 200 ns pulse [3], which is much more efficient than beam methods, but still insufficient for industrial implementation. Therefore, a logical direction is development of new processing methods for SiC, combining laser and plasma. In this paper, we demonstrate a new laser-plasma ablation method.
This work is devoted to consideration of the effect of ir nanosecond pulses (1064 nm, 200 ns, 1 mJ) on a 6H–SiC wafer (≈ 340 μm), which was located on a polished graphite substrate. The sample was transparent for the laser wavelength. When focusing into a 50 μm spot on the SiC surface or either on the graphite substrate, part of the radiation initiated the carbon plasma. As a result of using this technique, ablation craters were formed both on the upper and lower surfaces of the SiC wafer with a depth of 0.5–2 μm under reaction of the single pulse. A lower energy density was required for the appearance of silicon lines, which indicates a selective mechanism of SiC ablation by a near-ir laser. In addition, a C_2 molecule band (a system of Swan bands) was observed in the plasma plume, which can be explained by the recombination of excited carbon atoms both upon ablation of the outer surface of the SiC plate and upon ablation of a graphite target under the SiC plate.

[1] She X, Huang A Q, Lucía Ó and Ozpineci B 2017 *IEEE Transactions on Industrial Electronics* **64** 8193–8205

[2] Pawar P, Ballav R and Kumar A 2017 *Reviews on Advanced Materials Science* **51** 62–76

[3] Pecholt B, Gupta S and Molian P 2011 *Journal of Laser Applications* **23** 012008

About the mechanism of reverse deposition of titanium ablation products from laser erosion plasma

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The microrelief is formed on the titanium surface as a result of laser evaporation of it by nanosecond pulses. Wherein the surface of the microrelief is covered with a porous oxide layer formed by agglomerates of nanosized particles. The building mechanism of this layer is underexplored. Meanwhile, the formation of an oxide coating with a porous nanorelief is of great applied significance in the treatment of the titanium medical implants surface, since it promotes wetting by blood plasma and the attachment of proteins and other bioelements to the implant surface at the early stages of osseointegration. In the present work, the mechanism of nanorelief formation due to the reverse deposition of evaporation products after their oxidation in the atmosphere on the surface of the initial substrate is qualitatively considered. The chemical composition of the oxide layer has been studied. The relationship between the parameters of laser action during multipulse processing and the characteristics of the formed nanorelief is established. Theoretical estimates of the amount of back-deposited material are given as a function of the power density and duration of nanosecond pulses, obtained by solving the Boltzmann kinetic equation by direct statistical modeling.

Laser control of TiO_2-based nanocomposites optical properties

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Laser processing of nanocomposite materials paves the way to local and precise control of their optical properties. However for concrete applications such as integrated optics, photonic devices, photocatalytic devices, and security labels it is critical to know the exact relationship between laser irradiation parameters and optical properties of the resulted material. This study is aimed at local control of spectral characteristics of TiO_2 based nanocomposite thin films with Ag nanoparticles (NPs) carried out by a 405 nm diode continuous wave laser. In order to manage over the optical properties of such films, we changed scan speed and laser intensity. According to our experimental observations and numerical calculations based on the effective medium model, the mean size of Ag NPs and their size distribution differ within the laser track. A decrease of the scan speed, as well as an increase of the intensity, lead to a red-shift of reflection maxima at the edges of the track as a result of the mean particles size reduction and decrease of dispersion width. On the other hand, in the center of the track, a change in the reflection spectra occurs only at a laser power below 330 mW, where an increase in power leads to a shift of maxima to the blue region, which indicates a decrease in the mean size of NPs and a narrowing of their distribution. At a power above 330 mW, there is no change in the size and dispersion of NPs in the center of the track. These spectral dependencies are caused by different temperature distribution for different laser processing modes. The reported study was funded by the Russian Science Foundation, project No. 19-79-10208.

Hard x-ray focus characterization at the European X-ray Free Electron Laser using a fluorescent crystal detector

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Information upon the wavefront of x-ray radiation and its intensity distribution at the focusing point is extremely important for experiments that are carried out using x-ray free electron lasers (XFELs). In our experiments at the European XFEL, the focus of hard x-ray radiation was characterized at a High Energy Density beamline for the first time with using a LiF detector. Two compact refractive lens systems have been tested for achieving of μm–nm spot size. Due to the high spatial resolution (no less than 0.7 μm) and dynamic range (no less 10^6) of the LiF crystal, a real energy distribution of radiation and spot size in focus point were found.

X-ray diagnostics of laser-induced plasma embedded in strong magnetic field with misaligned orientation

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The present work is aimed at the experimental study of the dynamics of laser-induced plasma immersed in a strong poloidal magnetic field with variable orientation (0°–90° depending on the plasma expansion) and amplitude (up to 30 T). The significance of such studies is especially important for the tasks of laboratory astrophysics and inertial confinement fusion. Electron density and temperature profiles are measured, effects related with plasma collimation, accumulation, as well as separation, generation of instabillities and shocks by the magnetic field are discussed.

Optimization of laser plasma-based x-ray sources according to warm-dense-matter absorption spectroscopy requirements

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Recently [1], we discussed choosing optimum material and thickness of a target to get a bright x-ray source in the wavelength range of 2–6 Å (2–6 keV) considering relatively low-Z elements suitable for x-ray absorption spectroscopy (XAR) of warm dense matter [2]. In the present work, we demonstrated that the so-called photorecombination region of x-ray characteristic spectral emission is best suited for XAR using a laser-generated x-ray source, due to its featureless spectra of high intensity.

[1] Martynenko A S, Pikuz S A, Skobelev I Y *et al* 2021 *Matter Radiat. Extremes* **6** 014405
[2] Bressler C and Chergui M 2004 *Chem. Rev.* **104** 1781–1812

Method for precise wavelength measurements of middle-Z ions He- and Li-like satellites emitted by laser plasma of mineral targets

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In this work, an easy-to-implement method for accurately measuring wavelengths of spectral lines emitted by highly charged ions is presented.
It is proposed to use minerals of natural origin simultaneously containing elements with moderate ($20 \leqslant Z \leqslant 25$) and low ($Z \leqslant 15$) nuclear charge ($Z$) as laser targets. Emission from the latter ones provides perfect reference lines over a whole range of He- and Li-like moderate-Z ions emission under examination.
The method was implemented to precisely restore a dispersion function of a spectrometer with a spherically bent mica crystal as a dispersive element. As a result, wavelengths of dielectronic satellites corresponding to radiation decay of Li-like Potassium ions states were measured with precision 0.6 mÅ for the first time.
The reported study was funded by the Russian Foundation for Basic Research, project No. 19-32-60050.

X-ray spectroscopy diagnostic of iron plasma formed in experiments with ultra-relativistic femtosecond laser pulses in the case of pre-plasma formation control

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In this work, we present the results of x-ray spectroscopy diagnostics in an experiment with a J-KAREN-P laser facility for deliberate pre-plasma formation in steel foils, when a time-controlled femtosecond laser pulse was used for pre-plasma generation. The comparison of observed spectra of F-like and Ne-like Fe ions with results of kinetic modeling allowed to measure main parameters of plasma corona. We observed that plasma parameters mostly depend on natural sub-nanosecond laser pre-pulse, but fs-prepulse variation at the few-hundred picosecond timing becomes insignificant.

Particle acceleration and neutron production from submicro-sized targets irradiated by an ultrashort laser pulse

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In this work, the laser-initiated generation of thermonuclear neutrons in various submicro-sized targets irradiated by an ultrashort laser pulse has been studied using three-dimensional numerical simulation, using the previously obtained results of large-scale structural optimization of the target, which provides its best heating by femtosecond laser pulses of moderate intensity [1]. The report compares the efficiency of neutron generation from various targets including micro-wires, micro-layers (relief) on the surface of a flat foil, cylindrical micro-cavities and micro droplets. It is shown that, for modern laser technologies, femtosecond lasers of low (multi-mJ) energy are even more preferable for creating a neutron source than more powerful (1 J) lasers due to the practically available mode of high (1 kHz) pulse repetition rate.
The present work was supported by the Russian Science Foundation, project No. 17-12-01283.

[1] Gozhev D A, Bochkarev S G, Busleev N I, Brantov A V, Kudryashov S I and Bychenkov V Y 2020 *High Energy Density Physics* **37** 100856

Stochastic electron dynamics in microdroplet plasma irradiated by an ultrashort, intense laser pulse

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The use of submicro-sized mass limited targets in interaction with intense ultrashort femtosecond laser pulses is considered to be uniquely convenient approach for the development of a compact versatile pulsed source of secondary radiation. Innovative nano- and micro-sized targets, including droplets and micro clusters, allow effectively absorb laser energy, generate high energy electrons and, as a result, increase the production of accelerated ions, x-rays, neutrons, etc. In the case of the interaction of a laser pulse with nano- or micro-sized targets, the determining mechanism of a large energy gain by electrons is the stochastic heating in the combined field of the laser pulse and the Coulomb field of the droplets. We focus on study of hot electron generation and particle acceleration to energies beyond the ponderomotive limit. The model describes the high energy particle generation as a result of multiple elastic electron scattering on an expanding charged cluster. The expected appearance of supra-ponderomotive electrons should lead to an increase in the hardness of x-ray radiation.
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Neutron-shielding Al–B_4C coatings cold spraying from mechanical powder mixtures

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One of the urgent problems in the nuclear industry is the creation of new materials and coatings that provide radiation protection from thermal neutrons, which will make it possible to abandon the use of boron steels, which are extremely difficult and expensive to manufacture. In the present work, an experimental study of the properties of a composite neutron-absorbing Al–B_4C coating, formed using the method of cold spraying from a mechanical powder mixture of aluminum and boron carbide, was carried out. A series of coatings of different thickness was obtained with a boron carbide concentration of 23 vol % uniformly distributed in the metal matrix. The introduction of boron carbide particles into the aluminum matrix made it possible to increase the coating microhardness by about 1.5 times (from 46.3 to 71.6 $HV_{0.3}$). It was shown that coating with a thickness of about 1.7 mm is capable of absorbing up to 75% of neutron radiation, which is 14% more efficient than the currently used boron steel with a thickness of about 6 mm.

The results of investigation into the influence of plasma on electron beam parameters

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RNFC-VNIITF put the facility based on the linear induction accelerator (LIA) into operation in order to study dynamically developing objects due to explosive loading in the framework of pulse x-ray radiography method. One of the fundamental advantages of the LIA is the high-quality electron beam and small size focal spot. High energy release in the LIA target resulting from electron beam deceleration leads to formation of plasma torch that propagates towards accelerated electrons. This process has a negative effect on characteristics of the second and subsequent pulses in the multi-pulse mode of operation. In order to search and implement technical solutions on target plasma neutralization, one should be able to determine its parameters and record the dynamics of its propagation. At the same time, it is necessary to monitor the focal spot at each run using a diagnostic system that would not be positioned at the bremsstrahlung propagation axis. The paper presents the results of investigation into the target plasma propagation using the method of x-ray. The newly developed system for focal spot diagnostics in the negative direction and its principle of operation are described. The paper also presents the theoretical and experimental research on determining the LIA focal spot using the proposed diagnostic system by the "half-shadow of the sharp edge" method.

New insights in laser-driven ultra-intense gamma and particle sources for nuclear applications

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Ultra-high intense gamma and secondary particle beams are indispensable tools in many research fields like nuclear, atomic and material science as well as in high-energy density physics research. Especially for nuclear astrophysical applications, ultra-intense and high-flux gamma, neutron and proton beams are necessary to reach astrophysical scenarios in the laboratory. Such ultra-high fluxes of neutrons (in excess of 10^{21} n/(cm^2 s)) are unattainable with existing conventional reactor or accelerator-based facilities. Nowadays, concepts are discussed to generate neutron beams which are based on ultra-high power multi-petawatt lasers operating at $> 10^{23}$ W/cm^2 intensities [1]. Laser-driven relativistic electron beams are excellent tools for the generation of MeV gammas and particles. Here, it is presented a novel concept for the efficient generation of gamma and neutron beams based on relativistic laser interactions with a long-scale near critical density plasma at moderate relativistic laser intensities [2]. New experimental insights in laser-driven generation of ultra-intense well-directed multi-MeV beams of photons with fluences of $> 10^{12}$ ph/sr and an ultra-high intense neutron source with $> 10^{10}$ neutrons per shot are presented [2]. Optimization processes promises an ultra-high neutron fluence of $> 10^{11}$ n/cm^2 and corresponding neutron peak-fluxes of $\sim 10^{22}$ n/(cm^2 s) already at moderate relativistic laser intensities.

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High-current well-directed relativistic electron beams for multidisciplinary research

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High-current well-directed relativistic electron beam is an excellent tool for applications in many research fields such as plasma physics, nuclear physics, biology, cancer therapy, material science, etc. Pilot experiments performed at PHELIX-facility in Darmstadt as well as particle-in-cell and Monte-Carlo simulations demonstrated strong increase of particle and photon fluence in interaction of relativistic laser pulse with long-scale plasma of near critical density [1, 2].
In the presentation, current experimental results on electron, gamma and neutron generation as well as future experiments on applications in plasma physics and biophysics will be discussed.
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Laser-driven relativistic electrons for high energy density research

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The efficient generation of relativistic electrons with an energy of tens of megaelectronvolts in a plasma of near critical electron density was demonstrated at the laser intensities of (3–5) $\times 10^{19}$ W/cm^2 and a pulse duration of 1 ps. The collimated high energy electron beams reached effective temperatures that many times exceed those predicted by the ponderomotive Wilks scaling and carry charges of hundreds of nC. A good agreement between the experimental data and the results of the 3D-PIC simulations was obtained [1, 2].
Ultra-intense well-directed beams of MeV electrons and gamma-rays were generated at laser intensities that are relevant for the current short pulse high energy diagnostic lasers, e.g., at NIF and LMJ. Application of the low-density polymer foams will result in a strong increase of their diagnostic potential in probing of high energy density matter.
Acknowledgments: The reported study was funded by the Russian Foundation for Basic Research and ROSATOM, research project No. 20-21-00150.

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Synchrotron radiation as a tool for diagnostic of accelerated electrons dynamic in guiding structures

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Cappillary waveguides [1] or plasma channels [2] are known as effective tools for powerfull laser pulses propagation over many Releigh length and electrons acceleration by means of laser wakefield [3], or direct laser acceleration [4] regimes. Transverse betatron oscillations of accelerated electrons in quasistationary electric fields inside a guiding structure leads to emission of their synchrotron radiation. Estimations of parameters of synchrotron radiation spectrum (its characteristic frequencies, width and amplitude of spectral lines) can be used as a tool for diagnostic of electrons transverse motion. Particularly, it is shown, that measurements of the parameters of the synchrotron radiation spectrum can be used for diagnostic of parametric excitation of electrons betatron oscillations in guiding structures.

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Laser-plasma collider for accelerating electrons and positrons

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New laser-plasma methods of accelerating electrons and positrons is of great interest, since they can be used for new compact multistage accelerators up to ultrahigh energies unattainable by other methods using classical radio-frequency accelerators [1, 2]. High-quality beams of polarized electrons and positrons in the TeV energy range are required to carry out precision tests of the Standard Model [3, 4]. In this work, the developed and tested hybrid computational code [5,6], combining both PIC methods and grid methods, was adapted to simulate the acceleration process in separate stages of the laser-plasma collider of not only relativistic electrons, but also positrons. Each stage had a smooth entry and exit to ensure an adabatic change in the accelerating and focusing forces at the beginning and end of the acceleration process. The plasma profiles and channel shapes at the boundaries of the accelerating stages were studied to transport the particle beam between stages preserving its quality.

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Laser wakefield acceleration of a finite charge electron beam

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The interaction of a high-intensity femtosecond laser pulse with a rarefied plasma, the processes of wake wave generation and the acceleration of an externally injected electron beam in it are considered. The goal was to study the parameters of accelerated electrons, such as average energy, spread in energy, and acceleration length at which the minimum spread in energy is achieved, as well as to study the impact of the total charge of accelerated electrons on these parameters—the "loading effect".
For modeling, the developed WAKE-EXI code was used, which is a quasi-static cylindrically symmetric WAKE PIC code [1], modified to describe the acceleration of externally injected high-energy particles and the effect of their charge on the potential of the wake wave generated by an intense laser pulse.
The dependence of the before mentioned parameters of accelerated electrons on the electron injection energy is investigated. For test electrons (without taking into account the effect of the beam charge), good agreement with the theoretical estimate of the dependence of the optimal length on the electron injection energy is demonstrated. The dependence of these parameters on the value of the total charge of the electron beam is investigated. It was found that the electron beam charge is limited to a value of about 2 pC, provided that the relative energy spread should not exceed 2%.
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Production of quasimonoenergetic electron bunches in the interaction of a laser pulse with an inhomogeneous plasma

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In this work, the dependence of the characteristics of the ejected electrons on the amplitude of the laser pulse and the peak density of plasma electrons during the interaction of a laser pulse of subterawatt power with a plasma jet was studied. A method for obtaining quasi-monoenergetic electron bunches and increasing the energy of ejected electrons by varying the plasma density profile was proposed and tested.

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Mechanism of electron bunching by a relativistically intense laser pulse when crossing a nonuniform-plasma boundary

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The one-dimensional numerical simulation of electron bunch production in the passage of an ultrarelativistically intense laser pulse through a plasma boundary with a transition layer permits elucidating the main qualitative characteristics of this physical phenomenon [1]. As shown in the work [2], owing to the phase velocity variation of the wake wave produced by the laser pulse near the onset of plasma density plateau, there is a mechanism which favours a more intense bunch generation for the plasma with a diffuse boundary than for the plasma with a sharp boundary. As a consequence, the electrons that are accumulated in the bunch group more densely along the bunch length to form bunches with a denser head part. By separating out these electrons from the total set of bunch electrons, for the diffuse-boundary plasma it is possible to obtain bunches with characteristics which are superior to those obtained from the sharp-boundary plasma. By varying the plasma density and transition layer length as well as by selecting the cutoff energy, it is possible to control the bunch parameters and select the optimal values for the bunch injected into a laser-plasma accelerator.

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Benchmark experiment to prove the influence of projectile excited states on the ion stopping in plasma

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In this work, we report on a precision energy loss measurement and on our theoretical study of 100 keV/u helium ions in a hydrogen discharge-plasma. Collision processes of helium ions with protons, free electrons and hydrogen atoms are ideally suited for benchmarking plasma stopping-power models. Energy loss results of our experiments are significantly higher than the predictions of traditional models, where empirical values for the effective charge state Z_{eff} are used. We obtained good agreement with our data by solving rate equations, where in addition to the ground state, also excited electronic configurations were considered for the projectile ions. Hence, we demonstrate that excited projectile states, resulting from collisions, leading to capture-, ionization- and radiative-decay processes, play an important role in the stopping process in plasma.

Proton–boron fusion in a compact scheme of plasma oscillatory confinement

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We present the results of first experiments on the aneutronic fusion of proton-boron (pB) in a single miniature device with electrodynamic (oscillatory) plasma confinement ($p + {}^{11}B \rightarrow \alpha + {}^{8}Be^{*} \rightarrow 3\alpha$+8.7 MeV [1,2]). Device is based on a low energy (1–2 J) nanosecond vacuum discharge with a virtual cathode [3], the field of which accelerates protons and boron ions to the energies required for pB synthesis (100–300 keV) under oscillating ions head-on collisions. The yield of α-particles registered are presented and discussed in detail. The experiment was preceded by PiC modeling of main processes accompanying pB reaction within the framework of the full electromagnetic code KARAT [4]. Further studies are to show the prospects for the creation of a practical compact reactor on aneutronic pB synthesis with non-Maxwellian plasma [5] based on the oscillatory confinement.

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One-dimensional model of the indirect compression of targets under conditions close to the National Ignition Facility

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Within the framework of a one-dimensional model [1], which allows the analysis of experimental results, calculations of the compression of indirect targets were carried out, experiments with which are carried out at the National Ignition Facility (NIF) facility. The model is based on the RADIAN code. Spectral radiation transfer is considered in the multi-group approximation. In particular, the availability of an optical database makes it possible to use this program for analyzing processes in thermonuclear targets in which radiation is essential. The spectral absorption coefficients of radiation were calculated using the THERMOS program [2] (KIAM RAS). Numerical simulation of target compression was carried out, experiments with which were carried out at the NIF installation in 2011–2018 in various modes of a laser pulse, targets, hohlraum, as well as targets for the total laser energy NIF 1.8 MJ [3]. The model reproduces the data known from the literature on measuring the value of the radiation temperature in the cavity and on the velocity of the shells. The results of simulations using the one-dimensional RADIAN code are in the range of experimental results and LLNL calculations. The one-dimensional model correctly describes the process of compression of the target capsule and shows trends in changing the parameters of the target and laser pulse.

Localization and amplification of light in the explosion of porous-silicon-based composite

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Making silicon porous enables the creation of composite materials. Optically ignited, such composites show wavelength sensitivity and fast response. However, the explosion flash kinetics, especially at the period after reaching the maximum flash intensity, and its spectrum are still insufficiently explored. We demonstrate, that porous-silicon-based composites with perchlorate oxidizers exhibit a non-monotonic behavior of the explosion flash intensity. Approximately a millisecond after the explosive reaction start, the flash intensity plummets to zero for tens of microseconds, followed by simultaneous excitation of light and electromagnetic pulses. By changing the oxidizer, we found that a spectral position of light pulse 590 nm is independent of the perchlorate type. Our results suggest the unconventional self-formation of a random active medium consisting of silicon nanoparticles, where the localization and amplification of light may occur.

Quantum coherence versus thermal noise: Ultrafast Bose-like electron self-trapping in preheated diamond

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Ultrafast visible-range two-photon and carrier impact interband excitation of electron-hole plasma in natural monocrystalline diamond produces intense and unusual structured intra-gap uv-vis photoluminescence, representing electron self-trapping via multiple non-thermal transverse or longitudinal-optical (TO/LO) phonon emission as Bose–Einstein condensation-like process. The photoluminescence intensity increases versus laser pulse energy with steeply decreasing power slopes, indicating two-photon excitation balanced by self-trapping, radiative and Auger-recombination plasma dynamics. Stationary variable preheating of the crystal rapidly damps the non-thermal Bose-like self-trapping process through thermally-activated spontaneous emission of competing TO/LO-biphonon. Photo-injected free electrons gain additional kinetic energy through free-carrier absorption and can be resonantly trapped into narrow-band intra-gap energy states of luminous centers, exhibiting rich photoluminescence spectral structures of metastable phonon progressions, unattainable via direct excitation. The resonant carrier trapping mechanism reveals the unprecedentedly ultrafine vibronic features of the phonon-mediated relaxation dynamics in the intra-gap luminous centers, opening the way for their detailed structural studies, modeling and harnessing in quantum optics.

Impulse laser cutting of diamond accompanied by phase transitions to fullerene-type onions

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We studied a process of diamond cutting by a focused pulsed laser beam in an explosion inside solid matter mode (a 100-ns laser beam impulse focused in diamond generates a shock wave). A cavity size created in diamond by the laser impact is described by a conception of a blast cavity formation after explosion inside solid matter. Diamond cutting is also accompanied by a phase transition from diamond to fullerene-type onions composed of 2 to 5 shells. According to a new phase diagram of carbon [1, 2] (which contains a zone of diamond instability in the 55–115 GPa pressure range), the observed phase transition is possible under 70 GPa pressure and 2400 K temperature, which indicates pressure and temperature values during laser cutting. The pressure estimated based on the new phase diagram corresponds to the pressure estimated from the known blast cavity formation model.

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Threshold energy density studies at the laser ablation of the optical crystals for the ir spectrum

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The phenomena based on the laser ablation at the matter take a place in the modern technologies everywhere. These phenomena theoretical and experimental studies lay in the focus of our research work yet many years [1–5]. Modification of the crystals surface by the different chemical composition allows to change its optical properties in ir spectrum and to improve their strength characteristics. Further to the works [3, 5] the dependence of the threshold energy density F_{bn} at the laser ablation studies of the optical crystals (such a type $AgCl_xAgBr_y$ [6]) surface under the pulsed laser radiation with time duration of 20 ns on the such a samples beam strength have been fulfilled. The laboratory setup for the laser ablation of the studied samples was assembled on the basis of an experimental laser station in [1, 5].

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Optical breakdown of the oriented surface of sodium chloride

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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 oriented surface crystals of sodium chloride was studied [1].
In the case of femtosecond laser pulses, the main mechanism of the surface damage is thermomechanical ablation, which becomes the prevailing mechanism of radiative destruction of sodium chloride, if the duration of the laser pulse is less than 30 ps [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].
A threshold for laser destruction of the (110) NaCl surface was 1.5–2 times greater than that for the (100)-oriented surface [1].
This parameter have been determined surface energy [4, 5].
Information about surface energy (111) NaCl obtained [6].
It allows to estimate, that the threshold for laser destruction of the (111) NaCl should be higher than a side in 1.5 times, than for a surface (110), for experiences [1, 7].

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Study of mechanisms of second-harmonic generation of femtosecond laser pulse during plasma production in the presence of quasi-dc electric field

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In this paper, we investigate the mechanisms of the second-harmonic generation (SHG) during the interaction of the femtosecond laser field with gas in the presence of an external quasi-dc electric field. Based on the numerical solution of the time-dependent Schrödinger equation for hydrogen atoms, we find the ranges of parameters (intensity and wavelength) of the laser pulse, where the second harmonic is generated by four-wave mixing based due to the response of bound electrons or ionization-induced multiwave mixing due to the response of free electrons. In the latter case, the SHG occurs on the time scale of gas ionization (the growth of the plasma density), which is much shorter than the laser pulse duration due to the very strong dependence of the ionization rate on the electric field strength. Due to this, the parameters of laser pulses corresponding to the ionization mechanism of SHG are attractive for implementing sampling methods of measuring the waveforms of broadband terahertz radiation based on the SHG of probe laser pulse with variable time delay related to the terahertz field. The work was partially supported by the Russian Foundation for Basic Research (grant No. 20-32-70213).

Generation of mid-infrared pulses during interaction of two-color laser field with atomic clusters

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One of the promising directions for generating short pulses in the mid-ir range uses nonlinear multiwave mixing of two-color laser pulses with a frequency ratio close to two in a gas. In this case, mid-ir radiation is generated at the detuning of the higher frequency from the doubled lower frequency of the laser field. In this work, we show that the use of an atomic cluster gas can lead to the significantly higher efficiency of radiation generation at the detuning frequency as compared to the usually considered atomic or molecular gases. To do this, we numerically investigate the generation of ir radiation during the interaction of a two-color laser pulse with C_{60} fullerene using supercomputer numerical simulation based on time-dependent density functional theory. Based on a comparison of the results obtained for the C_{60} with the results for the hydrogen atom, it is demonstrated that the generation of low-frequency radiation in C_{60} is more than an order of magnitude higher than for hydrogen atoms at intensities corresponding to the same final degree of target ionization. The work was partially supported by the Russian Foundation for Basic Research (grant No. 20-32-70213).

Study of the nature of the effect of laser radiation power on Brownian motion in colloidal systems

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The results of an experimental study of the nature of the motion of a polydisperse emulsion system under the action of laser radiation of various powers are presented. The emulsion droplets were in an aqueous solution of the stabilizer and contained submicron carbon particles.
To study the nature of movement in the obtained emulsion systems, the droplets were exposed to laser radiation of various powers, their movement was observed using a stereomicroscope and recorded by a video camera.
As a result of processing the experimental video data for emulsion droplets, coordinates and velocities were obtained for each moment of time, kinetic energies were determined at various values of the laser radiation power, and graphs of the root-mean-square displacement versus time were plotted.
The movement of polydisperse drops of emulsions containing carbon particles was observed experimentally. Carbon particles can effectively absorb laser radiation, as a result of which the resulting thermophoretic force can set these particles in motion within the emulsion system, which in turn leads to the movement of the emulsion droplets themselves.
As a result of the analysis of the graphs of the root-mean-square displacement of the emulsion droplets and the dependence of the kinetic energy on the power density of the laser radiation, it was concluded that a change in the power of the acting laser beam leads to a change in the nature of the movement of the emulsion system.

Mechanism of active Brownian motion in emulsions of complex composition, induced by laser radiation

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Active Brownian motion in colloidal systems is an intensively developing topic, which is the subject of a large number of works [1, 2]. The study of active emulsions of complex composition, the mechanisms of their self-organization and the ability to self-locomotion will help to understand the essence of some similar mechanisms in cellular systems (especially the simplest unicellular organisms floating in a liquid).

Brownian motion in colloidal systems, which are quasi-two-dimensional structures made of polydisperse emulsion droplets of a complex composition, under the action of laser radiation has been studied experimentally. The results of the analysis of the trajectories of motion and the root-mean-square displacement of the emulsion droplets are presented. It was found experimentally that the droplet motion is active, including their motion observed in the superdiffusion mode. The mechanism of activity of emulsion droplets as a result of the appearance of motion when the droplets are heated by laser radiation is considered.

The present research was supported by the Russian Science Foundation (project No. 20-12-00372).

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New strategies of the hybridized carbyne-based nano-matrix spatially controlled growth during ion-assisted pulse-plasma deposition

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Structural self-organizing and pattern formation are universal and key phenomena observed during growth and cluster-assembling of the carbon-based nanostructures at the ion-assisted pulse-plasma deposition. Fine tuning these universal phenomena opens access to the properties of the growing nano-matrix. Taking into account that the sp1-bonds are formed only in a narrow range of optimal ion-assisted pulse-plasma deposition parameters, we consider the new strategies and technological tool-kit of the hybridized two-dimensional ordered linear-chain carbon nano-matrix spatially controlled growth and self-assembly. In particular, we propose combined application of the ultrasonic standing wave technology, which creates an acoustic hologram in the growth area and wirelessly powered discharge-induced electrokinetic phenomenon of the nano-matrix self-assembly. Existence of such phenomena was experimentally confirmed through the model experimental systems. We consider the influence of the acoustic waves frequency and oscillating electromagnetic field on the nano-matrix structure. We analyze the dependence of the nanostructures self-organization and self-synchronization phenomena from the ion-assisted pulse-plasma deposition parameters. We propose the data-driven carbon-based nanomaterials genome approach that is a new data-driven strategy for designing of the new carbon-based nanomaterials and forecasting of their properties. The reported study was funded by the Russian Foundation for Basic Research and TUBITAK according to the research project No. 20-58-46014.

Simulation of complex radiation action on aircraft constructions

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Due to the intensive development of generators of radiation and particles having various physical nature, it is required to design flying vehicles (FV) operating under the conditions of high-intensity energy fluxes [1]. The main method of confirming the strength to thermal and mechanical actions of radiation and particle fluxes is testing of full-scale aircraft structures to non-stationary loads from devices modeling these actions.

The work proposes new explosive devices and a unified test stand, which allows to model low-pulse mechanical action together with the thermal action. Thermal action is reproduced by contact electric heaters, high-power EHF emitters and pyrotechnic sheet charges.

A distinctive feature and advantage of the stand is the possibility to control the parameters of thermal and mechanical actions during the test. Such control is essential, since the reproducibility of these parameters when using explosive and pyrotechnic devices in some cases is insufficient. In particular, control is provided by the use of the ballistic pendulum technique to measure the momentum of the force transmitted to the tested construction. The design of the unified test stand takes into account previous developments [2], but a principal change has been made. Previously, heater and explosive device were exchanged by rectilinear movement. In the new version, the rotation of tested construction between heater and explosive device is proposed to use.

This work is supported by the Russian Foundation for Basic Research (project No. 19-08-00606).

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Effect of isothermal and electric pulse treatment on the structure of Ti50Ni25Cu25 rapid-quenched ribbons with a surface crystal layer

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In the present work, laminated amorphous-crystalline ribbons from alloy Ti50Ni25Cu25 with different crystal layer thicknesses were obtained by rapid-quenched technique on a rotating disk (planar casting method) at cooling rates of about 10^5 K/s. The amorphous-crystalline ribbons were subjected to heat treatment in a calorimeter, isothermal treatment in a muffle furnace (for 300 s) and electric pulse treatment with a processing time from 5 s to 1 ms. The processes of formation and growth of the crystalline phase from the amorphous part of the ribbon were studied using differential scanning calorimetry, scanning electron microscopy, and x-ray diffraction analysis. The microstructure of the ribbons after heat treatment in the cross section is characterized by an uneven distribution of crystals over the thickness of the ribbon: large crystals are present in the inner part of the ribbon, and on the contact sides columnar structures are observed. Electric pulse treatment with an exposure time of less than 1 s leads to a significant change in the formed crystal structure compared to the structure obtained by isothermal treatment. Columnar crystals observed from the contact side ribbon retain their original texture. With a decrease in the time of electric pulse processing, the proportion of columnar crystals that germinate from the ribbon surfaces to the inner part before their contact increases, and a homogeneous boundary is formed between them. This work is supported by grant No. 19-72-00145 from the Russian Science Foundation.

Applied studies in the framework of the Fundamental and applied Linear Accelerator Physics collaboration at the electron accelerator LINAC-200

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The electron accelerator LINAC-200 is a unique tool currently commissioned into operation at the JINR, Dubna, with a number of controllable parameters: electron energy in a range from 26 to 200 MeV (anticipated up to 2 GeV), macropulse duration from 30 to 3000 ns with a bunch duration of 1 ps, current from 0 to 60 mA, the capability of adjusting the pulse repetition rate in a range of 286–520 MHz. At present, this facility is the only one in the world with such flexible and reliably adjustable parameters. The high attractiveness of this facility to researchers resulted in the establishment of a new scientific collaboration FLAP (Fundamental and applied Linear Accelerator Physics collaboration). The FLAP collaboration is aimed at investigation of generation of electromagnetic radiation by relativistic electrons for deeper understanding of the nature of electromagnetic interactions and development of advanced diagnostic tools for accelerated beams of charged particles, spintronic devices and novel superfast detectors of electromagnetic radiation; understanding of the origin of CP violation in terms of new axion-like bosons; as well as a number of applied topics, such as nondestructive diagnostics of circulating and extracted accelerated particle beams, development of neutron detectors, pulsed neutron sources, radiobiological issues. The report addresses the development, testing and calibration of detectors based on microchannel plates for non-destructive diagnostics of accelerated ion beams, neutron detectors for applied research, including new concepts of energy production, pulsed neutron sources for studying extreme states of matter.

Prediction of J/psi, phi and D mesons production in the NICA energy range: Self-similarity approach

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The SPD (Spin Physics Detector) experiment is 1 of the 2 installations of NICA (Nuclotron-based Ion Collider fAcility) that is under construction at the Joint Institute for Nuclear Research, Dubna. It is expected that the SPD setup will provide physics runs after 2025. The J/psi production in hadron collisions is of great interest for several reasons. The description of the process is a challenge and an important test for our understanding of the quantum chromodynamics. Particles containing strange and charm quarks are important probes of the excited medium created in heavy ion collisions. Also, J/psi production, being sensitive to the gluon content of the colliding hadrons, would allow the study of gluon parton distribution functions. Thus, the SPD experiment is a powerful tool for verification of theoretical models and gaining deeper insight into the structure of matter. The SPD experiment is designed to ensure high precision measurements of total and differential cross sections and polarization with good particle identification. That is why it is extremely important to have reliable predictions for experimentally measured cross sections prior to planning experimental data acquisition routines. The presented functional self-similarity approach provides the construction of a solution quantitatively describing angular, energy and A-dependences of inclusive production cross sections for hadrons in relativistic nuclear collisions. It is applied for quantitative estimation of J/psi, and D meson production in the conditions of the SPD experiment at NICA accelerator complex with heavy and light nuclei. The results can be used for simulation of SPD detection system operation and optimization as a part of preparation for the physics run at the facility.

Magnetic-field influence on beta-processes in core-collapse supernova

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Neutrinos play a significant and sometimes even dominant role in all phases of the supernova explosion. The dominant neutrino processes in a core-collapse supernova are beta-processes, which are responsible for the energy exchange between neutrinos and the matter and change a chemical composition of a matter. We investigate an influence of a magnetic field on beta-processes under conditions of a supernova matter. For realistic magnetic fields reachable in astrophysical objects, we obtain simple analytical expressions for reaction rates of beta-processes as well as energy and momentum transferred from neutrino and antineutrinos to the matter. In our analysis we use results of one-dimensional simulations of a supernova explosion performed with the PROMETHEUS-VERTEX code [1,2]. We found that, in the magnetic field with the strength $B \sim 10^{15}$ G, the quantities considered are modified by several percents only and, as a consequence, the magnetic-field effects can be safely ignored, considering neutrino interaction and propagation in a supernova matter [3]. This work is supported by the Russian Science Foundation (grant No. 18-72-10070).

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Equilibrium radiation in plasma and plasma effects in cosmic microwave background

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In a recent paper [1], Munirov and Fisch proposed application of the well-known approach for the calculation of the fluctuation field radiation spectrum in a transparent plasma to the problem of cosmic microwave background. They used the result for spectral energy distribution of the equilibrium radiation, assuming that the spectrum of free photons is changed to the non-damping spectrum of transverse waves in non-relativistic plasma. The similar approach has been considered earlier by several authors for non-relativistic plasmas (see, e.g., [2] and references therein). The results of Munirov and Fisch are in fact in perfect agreement with the most of the previously existing expressions. However, we argue that this approach based on such simple approximation is not enough justified and the more elaborated consideration, taking into account not only temporal but also spatial dispersion of dielectric permittivity is necessary for a consistent description of radiation in plasmas. Moreover, interaction between free photons and charged particles in the framework of quantum electrodynamics leads to the result different in comparison with the standard consideration even for the transparent plasma medium [2]. The obtained new results for non-transparent plasma can be applied to astrophysical problems, e.g., the cosmic microwave background history, and also in Earth conditions, changing the asymptotical regimes for the spectral energy distribution of the equilibrium radiation.

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Gravitational anti-screenings around galaxies and dark matter halos in the composite supersymmetric superfluid quantum vacuum of the periodic waveguided multiverse

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Gravitational anti-screenings by virtual fermion–antifermion pairs—gravitational dipoles—are investigated in frames of the periodic waveguided multiverse (PWM) concept by the author. The PWM-concept expands the general relativity by Einstein and predicts the matter–antimatter (AM) gravity masses symmetry and the composite–weightless fermion–antifermion superfluid vacuum with the virtual gravitational dipoles. The gravitational anti-screening in this vacuum creates the gravitationally observed—invisible cocoon-like galactic halos around galaxies of ordinary matter (OM) or dark matter (DM) and increases their bare gravitational masses. The predicted PWM-DM-particles are intrinsically identical to OM-particles (very stable massive DM-photons, DM-electrons, DM-baryons, etc), living in two the nearest physically identical and literally parallel universes, they are detectable via OM–AM-mediating AM and creatable via AM–AM collisions. The PWM-vacuum concept simultaneously explains (a) the DM and dark energy (DE) mysteries; (b) reformulates the classical supersymmetry concept as the hidden–composite–unbroken vacuum supersymmetry, with zero cosmological constant by Einstein and (c) demystifies some basic QM-phenomena like the nature of probabilistic quantum-mechanical (QM) behavior, the double-slit experiment, the entanglement phenomena, Pauli exclusion and Heisenberg uncertainty principles in the QM.

The bodies of the zodiacal light: Their origin, evolution, and fallout

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Zodiacal light is a white cone of light that is visible in the west a few hours after sunset or in the east before dawn. Its location coincides with the ecliptic, the visible path of the Sun and planets against the background of stars. My article [1] considers the assumption that bodies of zodiacal light (BoZL) slowly drift along a set of horseshoe orbits, which were calculated by solving the three-body problem. Gravitational and centrifugal forces push the bodies away from the Lagrange points L1 and L2, so BoZL avoiding a collision with the Earth start the reverse motion along the horseshoe orbit. When BoZL cross the Earth's orbit their velocities reach their minimum values about 1 km/s, and their spatial density reach its maximum. This fact made it possible to estimate the total cross section of the set of these bodies about $(3\text{–}7) \times 10^{10}$ m^2. However, we failed to find out their distribution by sizes and masses. The article [1] considers two hypotheses. The first one suggested that the appearance of BoZL in the horseshoe orbits results from the scattering of fragments of the Giant collision [2]. Further evolution of BoZL in these orbits occurred due to their mutual collisions at velocities about several km/s. Multiple fragmentation of the BoZL occurred leading to the ionization of the environment by run-away electrons. Specification of their composition as well as the distribution by masses and sizes is possible by the means a space expedition along the Earth's orbit. This idea was first expressed by academician V E Fortov during my report at his seminar on 20 January 2020. The second hypothesis about BoZL fallout to the Earth was confirmed by magnetic studies of Antarctic dust [3].

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Luminescence of low-density two-dimensional electrons: Wigner crystal ore Mahan exciton?

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The many-body problem for 2-dimensional electron system (2DES) has no unified theoretical descriptions in the intermediate range of interaction parameter r_s neither for the ground state no for the elementary excitations. The ground state can be considered to be an electron gas, electron Fermi-liquid ore Wigner crystal (WC). High-quality MgZnO/ZnO heterojunctions have emerged as an excellent object for the study of electron-electron interaction effect in 2DES. The values of the interaction parameter r_s up to 10 are readily achieved. The photoluminescence spectra from the 2DES confined at MgZnO/ZnO heterojunction at r_s 6 are studied [1]. Electrons annihilate with the localized valence-band holes, and a quasiholes appear in 2DES. For the lower-density samples well defined lines from Landau levels depend unusually on magnetic field. In [1] this behaviour is connected with the phenomenon of the Mahan exciton [2]. The luminescence shape without magnetic field allowed both explanations: Wigner crystal and Mahan exciton. It is considered this work, that no unusual behaviour gives the taking into account Mahan exciton. For 2D Wigner crystal the Landau levels for vacancions depend differently on magnetic field from maximum and minimum sides of the band [3].

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X-ray spectropolarimeters and their application to Z-pinches

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X-ray spectroscopy is a powerful tool to study high temperature plasma which is effective source of He-like lines. There are number of models to describe intensities of He-like group so that comparison of experimental spectra with calculated one permits to extract plasma parameters. Models are not so trivial since pinch plasma is well known of its electron beam generated at the latter stage of the discharge. It means that time dependent modeling of spectra is required. Other effects should be taken into account in accurate way are: optical density, presence of electromagnetic fields, collisional exchange between levels, etc. Experiments carried out on Z-pinches have shown, that He-like lines are polarized. The reason for polarization are the presence of electromagnetic fields and (or) electron beams. Today the general recommendation is: first to analyze the degree of polarization of lines used for diagnostics, then chose the model to be used for their analysis. Study of polarized emission of pulsed plasma is important to get information on the physical processes in plasma, on the application ranges of conventional diagnostics approaches, it open perspectives to create new type of diagnostics. X-ray polarization analysis is based on the diffraction properties of crystals, where the integral reflection coefficient of ideal crystal testifies, that at Bragg angle equal to 45 degrees only sigma component is reflected and crystal serves as polarizer. Polarimeter is a device, which separates two mutually perpendicular polarizations. Polarization analysis of pulsed irreproducible x-ray sources is usually carried out with two identical polarizers or with single crystal polarimeter. This paper describes the design of two types of spectropolarimeters, which are intended to diagnose polarization of x-ray lines. The example of their application is also presented.

Heat transfer enhancement due to the spinodal decomposition of highly superheated solutions with the lower critical dissolution temperature

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Aqueous solutions studies are in demand when creating miniature cooling systems for electronic devices. Traditional liquid cooling systems are based on heat transfer intensification due to the liquid-vapour phase transition. However, in case of miniature heat exchangers application, local superheating and destruction of the heat exchanger due to the "dry" spots appearance in the course of vapour formation is not excluded. This research is aimed at studying spinodal decomposition, as a type of phase transition associated with the separation of the unstable solution (superheated with respect to liquid-liquid spinodal) into two phases of different composition. The object of study is an aqueous solution of polypropylene glycol (PPG) with an average molecular weight 725 pulse heated above the lower critical dissolution temperature.The report presents the following results of the study of aqueous solution PPG-725: phase diagram with binodal lines (experiment) and spinodals (calculation); coefficients of the instantaneous heat transfer to aqueous PPG solution in the regions of stable and unstable states obtained by the pulsed isothermal effect on substance. On the solution's phase diagram the region of spinodal decay is determined; it was also found that the instantaneous heat transfer coefficient of the solution significantly exceeded the corresponding value for pure water. This study was supported by the Russian Science Foundation (project No. 19-19-00115).

Characteristics of hemicellulose, cellulose and lignin pyrolysis

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Biomass is considered as a promising renewable energy source that includes all aquatic and terrestrial vegetation, waste from forestry, livestock and agriculture, or sewage. The organic part of biomass consists of three components: lignin, cellulose and hemicellulose. Its ratio varies depending on the type of biomass. The properties of these components have a great influence on the pyrolysis characteristics due to their different reactivity when exposed to temperature. The objectives of the project are to study the component composition of various types of plant biomass, as well as to study the interaction of organic components in the pyrolysis process, the effect of this interaction on the yield and composition of pyrolysis products. In the course of the study, data were obtained on the influence of the conditions for pyrolysis of the main components of plant biomass separately, in a model mixture and in the origin plant biomass. Slow pyrolysis at 350, 425, 500 and 575 °C was performed. The yield and composition of biochar, bio oil and pyrolysis gas at these temperatures were determined. This reported study was funded by the Russian Foundation for Basic Research, project No. 20-08-00835.

Experimental investigations on the effect of lignin, hemicellulose and cellulose interaction in plant biomass during pyrolytic treatment

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Plant biomass is a sought-after renewable resource for the production of synthesis gas, which can be used to generate heat, power or liquid chemicals. The study of biomass organic components interaction (lignin, hemicellulose and cellulose) during the pyrolysis is fundamental to a deep understanding of the transformation mechanisms, as well as to the possibility to predict the yield of liquid and solid pyrolysis products for various types of biomass. The technology of two-stage thermal conversion of biomass is an original method of producing synthesis gas and includes pyrolysis of biomass at 350–500 °C and gasification of the obtained biochar at 900–1100 °C using pyrolysis vapor-gas products as an oxidizing agent. The main scientific target of this project is to determine the common patterns of lignin, hemicellulose and cellulose interaction during pyrolysis in the first stage, which will optimize the second stage of the proposed method in accordance with the specific characteristics of the feedstock.

The reported study was funded by the Russian Foundation for Basic Research, project No. 20-08-00835.

Comparison of the effect of torrefaction and hydrothermal carbonization on biomass properties

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Today, one of the priority areas for the development of new methods of power supply is the elaboration of technologies for autonomous power supply of settlements. Energy utilization of waste, the main of which are wood and agricultural waste, solid municipal waste is a solution to the complex task of organizing local energy supply to settlements and eliminating accumulated environmental damage. The study considers the effect of heat treatment on woodworking waste (sawdust) in order to improve their thermal properties, including hydrophobicity. Torrefaction and hydrothermal carbonization were used as heat treatment methods. Torrefaction is a type of pyrolysis that occurs at temperatures of 200–300 °C in an oxygen-free environment, while hydrothermal carbonization (called wet torrefaction) proceeds at temperatures from 180 to 280 °C in the presence of water and without access to air. The main task was to study the thermal characteristics of biocoals obtained as a result of heat treatment.
The study was carried out by a grant from the Russian Foundation for Basic Research (project No. 20-08-00862).

Biomass self-heating energy using to increase the torrefaction process efficiency

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Agricultural, wood and woodworking waste utilization is an urgent problem, the solution of which is capable of protecting the environment, as well as a significant increase in the profitability of production in related economic sectors. Low-temperature pyrolysis (torrefaction) of biomass waste allows to produce high-quality solid hydrocarbon biofuel, which has higher rates of combustion heat value and hydrophobicity, which significantly reduces the cost of its transportation and storage. In addition, biofuels, being CO_2-neutral, do not upset the ecological balance. Torrefied product can be used as a fuel (either partially replacing coal, or completely as an independent fuel) in existing coal-fired boilers. However, despite the positive properties of the torrefied product noted above, its widespread industrial production is currently not implemented. The main reason for the lack of commercialization is the dearth of a competitive torrefaction technology, the availability of which would justify the high energy costs of producing a torrefied product. In the temperature range of 250–300 °C, typical for torrefaction, the main output is made by exothermic reactions associated with the decomposition of hemicellulose. An experimental quasi-continuous operating mode unit for low-temperature pyrolysis of granular biomass with increased productivity has been designed at the JIHT RAS. The unit makes it possible to partially use the heat of exothermic reactions occurring during the pyrolysis of plant biomass, which reduces energy consumption for torrefaction by a factor of 4–6 in comparison with the traditional approach.

Heterojunction with intrinsic thin layer photovoltaic panels operation: Numerical simulation and outdoor tests in Moscow

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Heterojunction with intrinsic thin layer (HJT) photovoltaic (PV) panels are known for many years [1], but large-scale production began only after Panasonic Corporation patent for this technology had run out of action [2]. Thin film layers of hydrogenated amorphous silicon, doped also with boron and phosphorus, provide additional amount of captured photons from different than for mono-Si part of solar radiation spectrum and less parasitic recombination due to excellent defects passivation. But energy yield calculation for such panel based on standard approach, involving PV panel standard test conditions parameters, have given less energy, than mono- and multicrystalline panels. Outdoor tests in Moscow conditions showed that HJT PV panels provide higher yield at low insolation conditions. So for proper HJT PV panel energy yield one needs to take into account solar radiation spectral composition. The approach to empirical coefficient deriving, based on comparative outdoor tests of different panels, is proposed.

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Infodemia as a new phenomenon in the COVID-19 era

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In the context of the development of a pandemic of a coronavirus infection, the flow of information on the problem of COVID-19 (COronaVIrus Disease 2019) is growing like an avalanche, which, according to the World Health Organization, has acquired the character of an "infodemic", which is a new phenomenon for society. The need for new data on a new disease can hardly be overestimated, but the overabundance of information that arose during the epidemic, which may or may not be reliable, makes it difficult to find reliable sources of information and recommendations when specialists need it. Like pathogens in epidemics, misinformation spreads faster and faster and makes it harder to respond to emergencies. How infodemic influences our decisions, what information about COVID-19 can be relied on, is modern medicine based on evidence or opinion, and what each of us can do to end the COVID-19 pandemic—these issues will be discussed.

2. Shock Waves, Detonation and Combustion

Numerical study of converging secondary shocks in neutrally-stable shock waves

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The two-dimensional analysis of the shock wave stability is known to predict the existence of neutrally stable shock waves [1,2]. The property of such waves is a weak attenuation of secondary waves, which are a superposition of acoustic and entropy-vortex perturbations in the space behind the surface of the shock wave, matched with the perturbations of the shape of its surface by relations on the shock-wave discontinuity (see, for example, recent studies of neutrally-stable shock waves [3, 4]. The behavior of converging secondary waves, accompanied by an increase in pressure and temperature in the hot region near the focus, remains outside the scope of two-dimensional analysis. In this work, we study this phenomenon based on the Euler equations in the framework of the three-dimensional formulation of the problem. It is shown that a decrease in the partial derivative of the internal energy with respect to the specific volume at a constant enthalpy for the post-shock state leads to an increase in the effect of cumulation of converging shock waves. Comparison of solutions for stable and neutrally stable shock waves is carried out.

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Behavior of porous matter along boundaries at the micro-scale under dynamic compression

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For shock experiments with porous matter the reflection method is widely in use. For calculations often the Mie–Grüneisen equation of state (EoS) is applied where a thickness of zero for the boundary surface between the reflector with higher impedance and the porous sample is used [1]. However, several experiments gave evidence that this assumption is not applicable. For the compaction of hard and brittle materials in the micro- or nanoscale and for the experimental work with powders the formation of a boundary zone during shock compaction is evident. It was shown with different analitical methods (optical and scanning electron microscopes, electron backscatter diffraction) that between the reflector material and the porous sample itself this boundary has a thickness of $\approx$ 10–20 μm. Within this zone intense structural, chemical and mechanical changes in both parts (reflector and sample itself) takes place. This concerns precompacted mixtures of different powdered materials too. The thickness of this area where an EoS lying between the reflector EoS and the sample EoS can be applied is nearly material independent. Because of the thickness of the boundary zone in the micrometer region, versatile impact for the compaction of powders with small grain sizes can be expected.

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Sound velocity measurement in shock-compressed fluoroplastic, epoxy resin and polycarbonate at 16–35 GPa

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In this work, three polymer materials were investigated (fluoroplastic, epoxy resin and polycarbonate). These materials, likely many other polymers, are utilized in airplane structure and used during gas-dynamic processing of special-purpose items. The study was aimed at obtaining the experimental data on sound velocity behind the shock wave front in the pressure range from 16 to 35 GPa in order to refine the equations of state of above-mentioned materials and to calibrate the existing mathematical models.

The paper presents the setups of explosive experiments and the data on sound velocity measurements in shock-compressed specimens of fluoroplastic F-4 (24–44 GPa), epoxy compound EC-34 (14–38 GPa) and polycarbonate PC-ET-3.5 (16–35 GPa) obtained by means of the rarefaction overtake technique. The photoelectric and the manganine gauge methods were used to measure sound velocity. The specimens were loaded by explosive loading devices based on powerful high explosives with steel impactor. The impactor velocities ranged from 2.7 to 4.8 km/s. The obtained experimental data is in good agreement with similar results obtained by other researchers within the experimental measurement error of 6–8%.

Experimental study of the viscosity of polymerized epoxy resin under shock compression

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The VISAR laser interferometry method was used to study the viscous properties of polymerized epoxy resin under shock compression in the pressure range 0.8–2.7 GPa. The Hugoniot is obtained in the coordinates mass velocity versus the velocity of the shock wave, which is consistent with the data available in the literature. The dependence of the maximum longitudinal strain rate on the pressure behind the shock wave front in the form of a power function is obtained. The value of the exponent 5.5 was significantly higher than the exponent 4, which is typical for most of these materials. The question of achieving a stationary propagation mode by shock waves in the performed experiments is considered. The viscosity coefficient of the polymerized epoxy resin is calculated, the values of which are in the range from 0.1 to 7.3 Pa s for the obtained shock compression pressures.

Shock-induced elastic, plastic and polymorphic transformations in iron films by picosecond laser pulse

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We present analyses of experimental and numerical studies of laser shock waves initiated by a picosecond pulse in iron. A very high deformation rate is a peculiarity of this research. It is important to understand how the deformation rate affects elastic-plastic and polymorphic transformations. The study of this problem is necessary for the development of a consistent theory of hardening of metals. A series of experiments were performed. Theoretical interpretation of experimental data is developed. Diagnostics of experiments only presents kinematics (free surface coordinate histories) of what is happening. Data on stresses is inferred to clarify the kinetics of polymorphic transformation. The transition of iron to the epsilon phase happens in the initial section of the propagation of the shock wave. Hydrodynamic and molecular dynamics numerical simulations verify theoretical approach for the inferred stresses.

Femtosecond laser-induced partial rear side spallation of bilayer Ni/Cr film

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Ultrafast chirped interferometry was used to investigate with the temporal resolution of 1 ps the rear side motion of the bilayer Ni/Cr thin film on a glass substrate under picosecond loading, generated by femtosecond laser pulse. The surface morphology after laser exposure indicates the presence of spall fracture at the contact of chromium and nickel layers. From the determined rear surface velocity history the value of the strain rate and the arising tensile stress are estimated.

One- to two-dimensional front crossover in laser-induced shock-waves modeling

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Laser induced shock-waves (SWs) have widespread area of applications nowadays. To most important of them belong laser ablation to liquids and laser shock-wave peening, where SWs are main drivers of physical and technical effect. Single femtosecond laser pulse action upon thick aluminium target is considered. SW generated after laser heating propagates in the target, firstly as planar wave and afterwards as hemispherical wave. Hydrodynamical simulations were made with different equations of state and different numerical methods to find and calibrate optimal hydrodynamic model and numerical algorythm for the phenomenon modeling. Attenuation of SWs is also considered and effects of ideal gas equation of state versus Mie–Grüneisen approach are analyzed. Results are compared to molecular dynamic simulations and experiment.

Dynamic plasticity of expanding copper cylindrical shells

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In the present paper, the features of the deformation behavior of Cu cylindrical shells expanding under the action of explosion products are investigated. The experimental statements in which different strain rates of the studied material are realized are described. In these experiments, the velocity of the shell were recorded electrocontact method, and to capture fragments of shells were used damping device, which managed to keep the shell elements for analysis. As a result of processing the experimental data, the plasticity characteristics—relative dynamic elongation and relative dynamic narrowing—were determined. The dependence of the relative dynamic constriction on the strain rate with a pronounced maximum, probably corresponding to the peak of plasticity, is obtained.

High speed photography of wire explosion in the distilled water

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Results of wire explosion experiment in the distilled water a presented. High speed photography was performed using Photron SA-Z high speed camera with the proper illumination. In order to calibrate the camera the metallic ruler was placed in the area between electrodes before the experiment. Shock wave speed and expansion rate if the gas bubble are measured and compared with previously measured [1]. Measured shock wave speed $D = 1474$ m/s is close to the value of 1470 m/s obtained in [1] in the same experimental condituions. Depending on the lighting conditions the shock wave appeared as shadow line or a mirror-like reflecting surface moving ahead the gas bubble. So we can conclude that there no instabilities on the shock wave front at least on the micron scale. Expansion rate of the gas bubble was also measured. It was 750 m/s which is twice lower than the shock wave speed. Bubble expanded with constant rate for 3 ms after wire explosion, than it starts to decelerate and collapse.

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Molecular dynamics informed neural networks for predicting the nucleation of dislocations and modelling of shock waves in thin metal films

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Increase in strain rate up to 1 ns^{-1} in the femtosecond laser experiments [1] can lead to homogeneous nucleation of dislocations. There are two main problems in the description of this phenomenon: a complex dependence of nucleation threshold on the loading path and non-linear variation of stresses at elastic stage. Artificial neural networks (ANNs) are used to describe the complex behavior of stresses and nucleation threshold, while molecular dynamics (MD) simulations are used for generation of data sets for ANN training. We reconsider nucleation theory and apply ANNs for approximation of material characteristics at elastic stage, which provides quantitative correspondence with the direct MD simulation of nucleation event. The nucleation threshold weakly sensitive to strain rate; it makes relevant direct approximation of nucleation threshold by ANN. It is shown that in the dislocation nucleation mode the elastic precursor of plane shock wave in thin Al and Cu films has constant height in contrast to decaying precursor in the dislocation multiplication mode. This work is supported by the Russian Science Foundation (project No. 20-11-20153) in the part of description of dislocation nucleation and by the Ministry of Science and Higher Education of Russian Federation (state assignment No. 075-00250-20-03) in the part of construction of ANN-based tensoral equation of state.

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Modeling shock-wave processes in face-centered cubic metals using the artificial neural network

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In the present paper, the artificial feedforward neural network was developed to approximate the equation of state for face-centered cubic metals. The data for learning the network was obtained from molecular dynamics modeling of the triaxial compression and tension Al, Cu and Al–Cu crystals. The obtained values of the weights and displacements of the neural network are needed to calculate the thermodynamic characteristics of a deformable material, such as pressure and internal energy, from the current values of density, temperature, and concentration of copper in an aluminum crystal. Plastic deformations emerging at the collision of metal plates were calculated using the modified Maxwell relaxation model. Dynamic loads can lead not only to deformation of the material, but also to cracking and destruction. Therefore, a fracture model was included in the simulation. This made it possible to describe the nucleation, growth, and collapse of pores in the sample under tension. The dynamics of the shock wave was investigated in a one-dimensional formulation in samples with various concentrations of copper. The results of measuring the velocity of the target free surface in pure metals were compared with the experimental data. The work is supported by the Ministry of Science and Higher Education of the Russian Federation (state assignment No. 075-00250-20-03) in the part of the equation of state and by the Russian Science Foundation (project No. 20-79-10229) in the part of the description of destruction.

Multiscale modeling of dynamical plasticity in Al–Cu alloy

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We combine molecular dynamics, theoretical model and discrete dislocation dynamics to investigate the dynamical plasticty of Al–Cu alloy. At the first stage we study the interaction of edge dislocation with various types of hardening inclusions of second phase in Al–Cu system, which are solute atoms, Guinier–Preston (GP) zones, θ'', θ' and θ phases. The main mechanisms of interaction between dislocation and different types of inclusions are established. It is shown that with an increase in the thickness of the hardening inclusion from one layer of copper atoms in the case of GP zones, the mechanism of the first interaction changes from cutting to the formation of Orowan loop. The accumulation of lattice incompatibilities upon repeated overcoming of an obstacle by a dislocation nevertheless leads to the gradual damage of inclusions. phase inclusions are the most stable. The parameters of the inclusion softening during long-term deformation are determined. Secondary, the model of dislocation-obstacle interaction is offered based on the concept of Orowan loop formation. The interaction energies for nanoscale hardening phases are determined by fitting to the moleqular dynamic data both for dislocation position and average stress in the systems. Inclusion softening is empirically taken into account by introducing an effective interaction radius that decreases with deformation. At the third stage, a discrete dislocation technique is formulated for plasticity modeling. Equation of dislocation motion accounts both dynamical effects and interaction with inclusions. The experimental data on size distribution of inclusions are introduced into the model. The obtained values of flow stress for alloy demonstrate good agreement with experimental results, also, calculations well predict the thermal softening of alloy.

Modeling of cylindrical shell collapse in finite deformations

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Experiments on collapse of cylindrical and spherical metal shells are used for researching the deformation behavior of metals in the conditions of energy cumulation in the converging shock wave. A significant experimental material has been accumulated currently [1]. This problem is of interest for the studying elastoplastic flows and destruction of the crystal structure of a metal at high strain rates and values. For example, the problem of collapsing metal cylinders implies that the material is underwent a relative deformation much greater than unity. To describe this process, the previously developed model of dislocation plasticity [2, 3] requires generalization to the case of large deformations.

We use the approximation of the results of molecular dynamics (MD) simulations for description of the behavior of aluminum sample. The dependencies between the stresses in a sample and his deformation are obtained from MD simulation. Approximation of these dependencies allows us to define the elastic component of deformation with using the deformation gradients and Green's deformation tensor. This approach allows us to solve wider specter of problems about propagation of shock waves in amaterials with ignoring the requirements of smallness of displacement gradients.

The work is supported by the Ministry of Science and Higher Education of Russian Federation (state assignment for researches by CSU No. 075-00250-20-03).

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High-speed collision of Cu profiled cylinders: Experiments and three-dimensional modeling using smoothed particle hydrodynamics, dislocation plasticity and artificial neural network-based equation of state

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A modification of Taylor anvil-on-rod tests is considered. Cylinders of 8 mm in diameter and 40 mm in length were cut from cold-rolled oxygen-free 99.9% M1 copper rod and machined in the head part to 3 different shapes: the reduced cylinder of 3 or 4 mm in diameter and 10 mm in length and the truncated cone with the top diameter of 2 mm and the length of 20 mm. The samples were launched by a gas gun with velocities from 19 to 78 m/s and collided with rigid anvil. The strains about 0.5 and the strain rates about 5/ms are realized in these experiments. In the case of reduced-diameter cylinders in the head part, the strain is almost equal through the length of the reduced part. The final form of the samples coincides well with the results of three-dimensional numerical simulation using smoothed particle hydrodynamics supplemented by the dislocation plasticity model. An equation of state (EOS) is obtained in the form of artificial neural network (ANN) trained by the results of molecular dynamics simulations. Experimental part of this work is supported by the Russian Science Foundation (project No. 20-79-10229); development of numerical code and ANN-based EOS is supported by the Ministry of Science and Higher Education of the Russian Federation (state assignment No. 075-00250-20-03).

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

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Investigation of metal alloys represent is a very relevant problem, because they are widely used for practical tasks. Solid solutions are of particular interest [1]. As shown in the previous work, the interaction of the edge dislocation with copper atoms in the aluminum solid solution can be represented as the interaction of dislocation with individual groups of copper atoms [2]. In this work, we consider the interaction between the edge dislocation and the cluster of copper atoms with various concentrations (20, 50, 80 and 100%) in the aluminum crystal. The aluminum single crystal has a size of $52 \times 60 \times 15$ nm^3 and crystallographic directions $[\bar{1}10]$, $[111]$ and $[11\bar{2}]$. The edge dislocation is created by inserting an atomic half-plane into the aluminum crystal, and the cluster of copper atoms with a size of 1 nm is created by substituted aluminum atoms in the dislocation path. The dislocation moves in the process of shear deformation, which is performed by the molecular dynamics method [3], where the interatomic interaction is described by the EAM potential [4]. The continuous model of this interaction process is proposed on the basis of previous works that study the interaction of the edge dislocation with structured inclusions [5].

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Atomistic and continuum modeling of the fracture of refractory metals

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In this work, using molecular dynamics (MD), we studied the kinetics of pore formation in the following refractory metals: tantalum, tungsten, and titanium. Representative elements of the volume of metals, both with an initially ideal lattice and with pores, were subjected to uniform triaxial stretching. The MD simulation was carried out using the LAMMPS program [1] and interatomic potentials for Ta [2], W [3] and Ti [4]. At the initial stage of preparation, the pressure was relaxed to zero using the barostat; the temperature at the stage of preparation and stretching was maintained using the thermostat (from 300 to 3000 K). The system was held for 10 ps. Then the barostat was turned off, and tension was applied at the constant strain rate of 3/ns. The pore number and size distribution were determined using an algorithm from [5]. The MD results were used to verify the continuum fracture model [6] and identify its parameters. At the stage of nucleation, an exponential pore size distribution is established.

Investigation of Ti and W is supported by the Russian Science Foundation (project No. 20-79-10229); investigation of Ta is supported by the Ministry of Science and Higher Education of Russian Federation (state assignment No. 075-00250-20-03).

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Modelling of spall fracture at high-velocity collision of metal plates

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Spall fracture at shock wave reflection from a free surface is one of fundamental processes limiting the dynamic strength of metals. Increase in strain rate considerably influence this process and increases the spall strength [1]; therefore, kinetics-based approaches are most suitable for its description at continuum modelling. The multiscale kinetic model of dynamic tensile fracture [2,3] is parameterized using molecular-dynamics data and implemented within one-dimensional finite-deference code. The modelling results are presented in comparison with the experimental data from the literature. The work is supported by the Russian Science Foundation (project No. 20-79-10229).

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Damage of titanium alloys under tensile at high strain rates

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In this work, a damaged medium model was proposed to describe the dynamic fracture of titanium alloys VT1-0, VT5-1 and VT6. The proposed model allows to describe both spall fracture and tensile fracture at high strain rates under conditions of a complex stress state. The elastoplastic response of titanium alloys is described by a constitutive equation taking into account the dependence of the flow stress from cumulative plastic deformation, homologous temperature, and the logarithm of the normalized equivalent strain rate [1].

The kinetics of damage was describing by parameter D as a result of nucleation, growth and coalescence of voids: $\mathrm{d}D/\mathrm{d}t = \mathrm{d}D_1/\mathrm{d}t + \mathrm{d}D_2/\mathrm{d}t$, where D is the damage parameter, D_1 is the constituent of D associated with damages caused by negative pressure, D_2 is the constituent of damages caused by voids evolution under repeated loading, $\mathrm{d}D_1/\mathrm{d}t = \alpha_1 \min[0, \mathrm{d}p/\mathrm{d}t]H(-p + p_c)$, where $H(\cdot)$ is the Heaviside function, p is the pressure, α_1, and $p_c < 0$ are constants of the material, $\mathrm{d}D_2/\mathrm{d}t = [1/(\gamma_1 A\sqrt{2\pi})] \exp[-(\ln(A)/\gamma_1\sqrt{2})^2]$, where $A = \int_0^t W^e[\beta_1 \exp(-\beta_2 W^p)(1-D)]^{-1}(\mathrm{d}W^p/\mathrm{d}t)\mathrm{d}t$, β_1, β_2, γ_1, are constants of the material, W^e, and W^p are the specific internal energy, and the specific dissipated energy, respectively. Obtained results of numerical simulation are in agreement with the available experimental data on a spall and dynamical fracture of titanium alloys. It was shown that in spall zone there are meso-volumes in which the alloy has undergone severe inelastic deformation. These inelastic strains occur during repeated loading of the alloy in reflected loading and unloading waves. The work is supported by the Russian Science Foundation (grant No. 20-79-00102).

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Analysis of the high-speed strain of the solid and volume-periodic samples of aluminum grade AK6, made under the additive technology within the range of rates 10^2–10^3 s^{-1}

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The samples having both solid (homogeneous), and volume-periodic structure were studied during operation on the split Hopkinson pressure bars (SHPB) installation. Loading experiments using SHPB technique allow to obtain dynamic compression tensile diagrams within the range os strain rates $\varepsilon = 10^2$–10^3 s^{-1}.

The work objective: investigation of dynamic properties of the samples made using additive technologies. Problem: obtaining of dynamic strength characteristics and the analysis of the experimental data resulting from the series of experiments on SHPB installation with three-dimensional (3D) samples of aluminum grade AK6 at the strain rates from 5.5×10^2 to 37.0×10^2 s^{-1}.

Samples made of aluminum having the same chemical composition as alloy AK6, of the set volume-periodic structure were made by selective laser sintering of metal powder on industrial 3D printer.

More than 60 experiments were performed. Stress–strain diagrams and strain–strain rates within the range of impactor velocities from 7.14 to 31.2 m/s were obtained, thus own strain rates of samples were from 8×10^2 to 37×10^2 s^{-1}.

Stimulated Mach configuration generated by intense heavy ion beam as a scheme for investigation of high energy density matter

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In frames of HED@FAIR collaboration for experimental study high-energy-density (HED) matter in extreme state created by intense heavy ion beam were proposed schemes LAPLAS and HIHEX. Another scheme Stimulated Mach Configuration (SMAC) 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 stem of Mach wave HED matter region with practically 1D hydrodynamic motion suitable for experimental research. Results of numerical simulations of hydrogen compression in LAPLAS and SMAC schemes are compared.

Simulation of Richtmyer–Meshkov instability in solids via smoothed particle hydrodynamics

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The shock loading of solid samples which have perturbations on the free surface may lead to the development of Richtmyer–Meshkov instability [1,2]. It was demonstrated recently [3–5] that the analysis of such flow allows to define shear and yield properties of material at extremes. According to the experimental studies we perform simulations using the smoothed particle hydrodynamics method. The two regimes are analyzed: the light shock load, when only limited growth of perturbations is observed, and the heavy load leading to an unstable growth of jets from the free surface. In the first regime we noticed that shear waves can propagate along a corrugated surface causing the low-amplitude harmonic oscillations of the surface. A good agreement of the oscillation period with the theoretical dependence [3] is demonstrated. The possibility of using simulations to assess the strength of tantalum according to [5] is also analyzed. In the second regime the jet velocities obtained in simulations of copper samples loading are in a good agreement with the experiments [4].

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Experimental study of shock-wave properties of emulsion matrix at various values of filler concentration

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The present study considers an emulsion being an aqueous solution of ammonium nitrate with mineral oil and an emulsifier. The emulsion matrix density was $\rho_0 = 1.35$ g/cm^3. The samples porosity was controlled by adding glass microspheres with an average diameter of 70 μm to the matrix.

The authors studied three types of emulsion matrix samples featuring various filler concentrations, the latter being 1, 3 or 4% by mass. The samples density was 1.25, 1.07 and 1.025 g/cm^3 accordingly. The mass velocity profiles were recorded with VISAR laser Doppler interferometer.

The experimental data, when processed, resulted in a Hugoniot of the emulsion matrix, the maximal pressure being 35.2 GPa. This Hugoniot was well approximated with the generalized Hugoniot for liquid media. The Hugoniots of the porous samples were determined up to such pressure values, which, when exceeded, initiated a chemical reaction in the medium. The relative position of the Hugoniots featuring different filler concentration was typical for porous media. In particular, in the vicinity of 3% there occurred a change in the curvature of the relationship between shock-wave velocity and mass velocity.

At low pressures, the compression-pulse structure in porous samples had typical blurring of the shock-wave front while the wave was propagating through the sample. For instance, if the sample thickness changed from 4 to 8 mm, the material with 4% filler concentration had a shock-wave front that became more than three times wider than before, reaching several microseconds.

Calculation of shock adiabats of mixtures at high pressures

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In this work, we calculate the shock adiabats for mixtures of different materials. The calculation is based on the additivity method of shock adiabats of components, according to which, at a given shock compression pressure, the specific volume of the shock-compressed mixture is the sum of the specific volumes of the shock-compressed components of the mixture, taking into account their mass fractions. The results of this calculation of shock adiabats are compared with the available data of shock-wave experiments for two-component mixtures and alloys at high pressures.

Method of multiframe holographic registration of high-speed processes

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In this report, a method of the multirame holographic registration of parameters of microparticles, which appear on a surface under a shock wave, is presented. The method is based on a digital rotating mirror camera and it is allows receiving sequence of holographic images with time interval 1 μs on full frame image sensors.

Study of products of slow thermal decomposition and explosive conversion of benzotrifuroxane, triaminotrinitrobenzene and trinitrotoluene

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To a large extent, the efficiency of the reaction products of energy-intensive compounds depends on the directions of chemical reactions and the conditions of their initiation. It is obvious that the thermochemical and gas-dynamic properties of reaction products are the most valuable for technical physics and the applied use of high explosives. In addition, information on the composition of chemical reaction products under slow thermal decomposition conditions and their properties allows us to assess the storage and operating conditions of energy-intensive compounds, as well as compatibility with various materials. In this paper, complex studies of the composition of products of slow thermal decomposition and explosive transformation of benzotrifuroxane, triaminotrinitrobenzene and trinitrotoluene are carried out. The sources of ultrapure samples were obtained by sublimation method. The purity of the studied substances was confirmed by high-performance liquid chromatograph mass spectrometry (HPLC/MS), Fourier transform infrared (FTIR) and Raman spectroscopy and powder x-ray diffraction.

Research of products of slow thermal decomposition and explosive conversion of cyclotetramethylene tetranitramine, cyclotrimethylene trinitramine and dinitroanisole

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From the chemical point of view, technical properties of high explosives (HEs) depend on the directions of the reactions of interaction between the components and the conditions of their initiation. The most valuable technical and applied characteristics of energetic substances are the thermochemical and gas-dynamic properties of reaction products. In technical physics, information about the composition of chemical reaction products under conditions of slow thermal decomposition and explosive transformation is used, which is estimated according to physical and chemical studies and theoretical modeling. In this work, carried out comprehensive studies on products of slow thermal decomposition and explosive transition cyclotetramethylene tetranitramine, cyclotrimethylene trinitramine and dinitroanisole. As a result, the equations of chemical reactions of the processes of slow thermal decomposition and explosive transformation are compiled. The thermochemical and gas-dynamic properties were evaluated, and data were obtained for constructing equations of state for the reaction products of HE in various interaction modes.

Tidal effects on companion with lower mass in a binary neutron star

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Present report deals with tidal effects on lower-mass component in a binary neutron star. Tidal destruction of the component due to loss of mass to tidal forces are of particular interest. A recently proposed equation of state of dense matter was used to evaluate density distributions in low mass neutron stars and Rosh limits in binary stars with uneven mass distributions. Classical approach was employed. Results of hydrodynamic simulations of tidal destruction of lower-mass component are also presented

A wide-band microwave radiation generated by high explosives

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Several experimental facts shown, that microwave radiation (10^8–10^{11} Hz) is generated during high explosive (HE) charge detonation process, with charge weight being $M = 10^2$–10^4 g. The radiation intensity exceeds an intensity of thermal radiation. In the process of expansion of HE products the concentration of electrons behind a shock wave decreases, and microwave radiation falls outside the limiting resonator. The mechanism of radiation [1] will take effect after some delay from the moment of HE initiation, and this delay time is proportional to HE weight. If nonlinear effects is absent, the average frequency of radiation should decrease during a pulse. A type of HE, a charge geometry, existence of a shell, a way of initiation, as well as external pressure are the important parameters, influencing on the mechanism. To obtain wide-band microwave radiation, the optimal HE composition should be used. The radiation should be registered with a certain delay. The delay depends upon the moment, when the detonation wave comes on the charge surface. Our recent experiments demonstrated time delays in agreement with the mechanism.

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A magnetic cumulative generator with opening switch

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Experiments with magnetic cumulative generators were carried out, and inductive loads 1 μH used. 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, the pulse leading edge was no more than 4 μs. Intercepted magnetic flux in a primary circuit was 0.08 Wb. The output current pulse was 0.38 MA, and the coefficient of flux conservation 0.614. There is a limitation because of maximum high electric field in the generator, thus overall performance of magnetic cumulative generator cascades was taken into account. A numerical simulation of such generators depends on a lot of non-linear parametric data, which can be received from special tests. The experiments under consideration have demonstrated a high performance and effective application of the small-sized devices for impulse magnets supply.

The influence of physical, chemical and technological characteristics of high explosives on their shock wave sensitivity

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The given work presents results of investigations of the shock wave sensitivity of high explosives (HEs) in gap-test set-up. They performed assessment of the influence of their physical, chemical and technological characteristics on the level of shock wave HE sensitivity. The experiments were performed on the cylindrical samples of plastic and thermoplastic HE based on octogene, TATB, hexogene and finely-dispersed ten. They used the values of time delay and the depth of detonation origin, that at the same time characterize detonation HE capability, as the criterion of assessing shock wave sensitivity for this method. Determination of the time delay and the depth of detonation origin was performed using recording techniques such as electrical contact, radio interferometric and photo chronographic techniques simultaneously. Due to different initiating capability of above mentioned HE they developed shock wave generator permitting to vary the pressure of the wave, arriving to HE sample in the interval 30–60 kbar. It was found that the density, sorption specific surface and porosity of HE granules can influence on the valve of time delay for detonation origin. Besides the density of HE samples can influence on level of shock wave sensitivity, and existing axial HE samples inhomogeneity may cause the change of time delay of detonation origin by 10%.

Determination of shock wave parameters under explosion of high-explosive charge

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Developing high-explosive (HE) compositions, it is necessary to assess the level of their power under conditions of an explosion in air. As a rule, in order to assess HE power they use such characteristics as maximum residual pressure P and pulse of compression of positive phase I for air shock wave (SW). While determining these characteristics, they usually apply various pressure gauges, timers and impulse meters. Besides certain requirements are imposed upon preparation of the working field, where experiments are performed. The goal of the current work was determining the parameters of air SW under the explosion of HE charges by registration of gas luminosity at SW front without using pressure gauges and timers. The object of the investigations were experimental nodes (EN) that were fabricated out of trotyl, phlegmatized octogene, hexogene and TATB (triaminotrinitrobenzene). In these investigations shifting of air SW front was tracked by registration of air luminosity at its front. They built the dependence of SW front passing on time (x–t), with the help of which parameters of velocity and residual pressure of air SW were determined for HE under study. Experiments used digital electron-optical camera and high-speed photorecorder intended for registration and measurements of fast running processes in one-frame mode and the mode of line sweep of the image under study. The principal possibility of finding the characteristic P with the help of electron-optical camera and high-speed photorecorder without using pressure gauges and timers was shown.

A factors of the unstable initiation and propagation of combustion waves in thermite mixtures

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Effects of the porosity, the energy of electric spark initiation and the diameter of the linear channel upon the formation of a combustion wave in thermite mixtures $Al + CuO$ and $Al + Bi_2O_3$ are studied. Photos of the combustion wave propagation in a channel with transparent walls show spatial inhomogeneity of radiation. In a number of experiments, before the constant velocity value is established, the dynamics of the frontal part of the combustion region has an exponential character of development. In experiments with opaque dielectric walls, the current was measured across the local reaction region. The dynamics of electrical conductivity in the front of the combustion wave is oscillatory in nature against the background of its value growth, which can also be approximated by an exponential function. At low currents through the initiating spark or a small charge diameter, combustion collapse occurred. At the same time, a spotty structure of the cross-section of the unburned mixture was observed, and characteristic signs of reaction intermediates were observed on the channel walls. With a more complete combustion of the mixture, the final products of the reaction were mainly found on the walls of the channel. The increased porosity of the mixture in the channel increases the filtration rate of hot intermediates, but increases the probability of combustion collapse. The report discusses the influence of the mixture, initiation and channel parameters on the detected trends in the combustion wave dynamics.

High velocity regimes of plasma propagation supported by laser in condensed and hollow silica-based optical fibers

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This work has been done by the Joint Institute for High Temperatures (JIHT RAS) and Fiber Optics Research Center (FORC RAS). We had investigated ultrafast self-contained regimes of plasma propagation supported by laser in condensed and hollow silica-based optical fibers. Damage of the light conductivity in media of optical fiber transporting intense laser energy leads to the absorption of this energy and the appearance of a bright laser plasma. The created plasma begins to move towards the radiation source, irreversibly damaging the light guide. Experimental results were obtained for condensed [1–5] and hollow optical fibers [6, 7]. Key physical processes in both types of silica optical fibers are discussed.

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Initiation of detonation by shock wave in flammable gas containing inert particle

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Particle interaction with shock wave changes the fluid properties in the vicinity of the particle. The bow shock reflects backward from the front side of the particle. Between the bow shock and particle, the subsonic region is arisen. Gas becomes hot and compressed in the subsonic region behind of bow shock front [1]. It is shown in [2] that the danger of initiation of detonation appears when combustible gas shock encounters even the single 100-μm particle. In work [3], detonation limits for shock in hydrogen–oxygen mixture with solid particle suspended in fluid were obtained numerically. In all our previous work the particles were assumed to be adiabatic. Main idea of our work is to improve understanding of details of regimes, which potentially enable to initiate the detonation. We have investigated the heat disturbance caused by the particle and in the present work, we have focused on study of heat conduction and heat accumulation in the particle and how the heat absorption effects on the fluid properties. Data on energy balance between the particle and gas fluid are necessary for clarification of detonation limits with taking into account of described process. The spatial and time limits of used methods are determined.

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Analytical method of adiabatic curve plotting for explosion products expansion based on the cylinder-test experiment

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Process of work performance upon the environment under detonation and also shock wave profile generated in the environment for each high explosive (HE) are uniquely determined by the equation of state for explosion products (EP). Equation of state for EP explosive is determined based on the adiabatic EP expansion passing through Chapman–Jouguet point. Shock wave parameters in the reference materials contacting to an edge of detonating HE charge are usually measured for definition of the run of the adiabatic curve in the Chapman–Jouguet point region. HE propellant force experiments are performed for determining EP isentropic expansion in the low pressures range (in the order of 1–10 GPa). So experiments of edge throwing of the plates by HE explosion products are widely used.

This work presents the analytical method of the obtaining of the adiabatic curve of detonation products expansion directly from experimental data on cylindrical shells scattering, throwing by explosion products of detonating explosive. While plotting EP adiabatic curve, the shell incompressibility and its density stability during movement under the influence of explosion products were assumed. Adiabatic curves of explosion products expansion of the low sensitive HE for various initial HE radii were plotted.

Numerical modeling of combustion and electrization processes in a solid-fueled ramjet afterburning chamber

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A numerical model of internal processes in a solid-fuel ramjet combustion chamber was developed. The model takes into account two way interaction between fluid and condensed phase (particles of aluminum diboride, AlB_2) during stages of ignition and combustion. The electrophysical effects caused by chemical ionization of gas and the charging of dispersed phase were considered. The temperature and velocity fields of the high-speed two-phase flow in the ramjet afterburning chamber were determined in dependence of the particle size of the condensed phase, the air-to-fuel ratio and the initial parameters of the air flow. The electrical charges of moving condensed phase particles were calculated based on a thermionic emission model. The verification of the suggested model was performed, which showed the reliability of the obtained data and an acceptable level of accuracy. This work was supported by the Ministry of Science and Higher Education of the Russian Federation (project No. 0705-2020-0044).

Investigation of flames of methane–air mixtures stabilized on a flat porous burner

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In the present work, we studied the structure of methane–air flame in different combustion modes. For this, a flat porous cylindrical burner with a diameter of 15 mm was created. The burner contains a part with a porous filling and a set of capillaries with an inner diameter of 0.2 mm. The temperature distribution in the flame was measured by fine-fiber pyrometry for stationary combustion modes. The resulting data represent calibration measurements for further comparison with coherent anti-Stokes Raman spectroscopy temperature measurements.
The measurement of the dependence of the molar concentration of the OH radical on the distance to the burner surface has been carried out. The measurements were carried out using the laser induced fluorescence (LIF) technique. Excitation wavelength 281 nm [transition A–X (0.1)], registration of the LIF signal at a wavelength of 313 nm [transition A–X (0.0) and (1.1)].
The experimental results were compared with the data obtained by direct numerical calculation based on a model with a detailed GRI reaction mechanism.

M-flame under external acoustic field

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The trend towards permissible reduction of NO_x emission standards requires the development and implementation of conceptually new technologies in the energy industry. Combustion technologies improvement methods can be divided into the following groups: lean mixtures combustion, catalytic combustion, and two-stage combustion (rich combustion—rapid mixing with an oxidizer—poor afterburning). Premixed lean combustion is the most commonly environmentally friendly technology used in the modern energy industry. However, such combustion less stable in comparison with diffusion one. Often, lean combustion systems operate under near-limit conditions. And, even insignificant fluctuations in the mixture composition, operating parameters, geometric configuration, and the method of introducing reagents can lead to a significant change in heat release and a possible resonant increase of the flame oscillation intensity. Typically, this resonant amplification is caused by the effects of acoustic vibrations present in most technical devices. In this case, the elements of the device that are not directly related to the functioning of the burner unit can also serve as the primary source of acoustic vibrations. Typical design solutions of burners and combustion chambers of engines are often subject to the formation of the above-described positive feedback, including due to the transmission of acoustic vibrations along the structure. Such flame instabilities, excited by acoustics, are referred to in technical devices as thermoacoustic ones. The current study is devoted to the stabilized premixed flame characteristics under the external acoustic field.

This work was supported by the Russian Science Foundation (grant No. 20-79-10328).

Image processing for analysis methane–air flame front dynamics

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Excessive NO_x emissions are a serious problem in modern combustion chambers. Using premixed mixtures with a low equivalence ratio is a promising technology used to reduce NO_x emissions. However, the premixed flame is less stable than diffusion flame. Therefore, it is necessary to develop methods that increase stability. To understand the instabilities nature first step is to study the flame front dynamics. There are various methods for its study [1], but the analysis of chemiluminescence flame images has advantages over others: high reliability and versatility. A universal effective technique for the flame front contour extraction as a 1-pixel continuous line is proposed using chemiluminescence flame images. The technique consists in the sequential application of filters. The effectiveness of the method was tested on the high-speed images analysis under various premixed flame parameters. The versatility is ensured by the automatic selection algorithm of the "Canny" filter parameters using the original image. The implemented filters helped to solve main processing problem caused by the inhomogeneity of the glow flame front intensity [2]. This paper presents the results of image processing with using this technique. Estimates of the flame front oscillations were obtained for various combustion modes.

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Gravity impact on swirled flame stability

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It is known that the structure of non-reacting swirling jets substantially depends on the degree of flow swirling and the method of its imposition. With a sufficiently strong swirling in the mixing layer, spiral instability modes are enhanced, the vortex core decays, and a recirculation zone appears. In this case, the decay of the vortex occurs in various forms: spiral, bubble and (or) conic. In the case of reacting swirling flows, the effects of thermal expansion are superimposed on top of all the above-described effects. Accordingly, in practice, flow swirling is used as a method for the formation of large-scale vortex structures. Such structures provide for the existence of stagnant recirculation zones, which make it possible to increase the contact time of the reaction products with the fresh fuel–air mixture. During contact, the fuel–air mixture is heated, which facilitates its ignition, in turn, the precession of the vortex core significantly increases the intensity of heat and mass transfer. All this increases the stability of combustion, especially lean combustible mixtures. It is known that gravity through the forces of buoyancy makes a notable contribution to the dynamics and stabilization of the flame. In this case, the lower the flow rate, the more significant the influence, since there is competition between the buoyancy forces and the flow pulse. Earlier, it was shown that swirling flames take on different shapes under normal and reverse gravity. This work is devoted to the analysis of the stability of swirling methane–air flames depending on the direction of the action of gravitational forces. The shape of the swirling methane–air flame under the different fuel equivalence ratio conditions and gravity are studied.

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Methane–air flame stability under the various gravity conditions

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Flame stabilization under various gravitational conditions is critical for a wide range of applications. In laboratory experiments, a conical flame is most useful. Experimentally, the stability of an inverted conical plane-symmetrical premixed methane–air flame under normal and reversed gravity was investigated. The flow velocity was varied from 1 to 8 m/s, and the fuel equivalence ratio was varied from 0.8 to 1.4. Depending on the set of conditions, such a flame could be V-shaped (attached only to the stabilization rod) or M-shaped (attached both to the nozzle edge and the stabilization rod). Under normal and reversed gravity, the transition between two modes was studied. The hysteresis properties of the M–V and V–M transitions in normal gravity were reported, as well as their absence in reverse gravity. At the maximum burning velocity, the most unstable flames were observed under reversed gravity ($\phi \approx 1.1$). Under normal gravity, a reverse flow exists above the stabilizer at any velocity, and under reverse gravity, at high velocities (> 5 m/s). With increasing velocity, the longitudinal size of the vortex zone increased linearly in both cases. Gravity was found to play a significant role in the stability of rich flames.

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Stability limits for methane–air flames under the external acoustic and gravity impact

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Recently, methane has become an important fuel for power plants. This is due to the advantages of methane as a fuel: low cost, relatively high density, environmental safety, proven storage technologies, etc. However, the creation of stably functioning methane engines requires solving a number of fundamental problems associated with a narrow concentration range of ignition, as well as a low methane–air reaction rate. During the real aircraft operation, external effects affect the flame, such as gravity (due to maneuvering), acoustic effects that can provoke its destabilization and blow-off or flash-back, which can leads, to severe consequences, up to the engine and aircraft destruction. Lean flames stabilization can be implemented using stabilizing bodies that promote vortex flows formation. In the vortex flows region, the velocity decreases, which makes it more sensitive to the mass forces effect (in the case of subsonic flows). Similarly, acoustic disturbances affect the vortex flow nature, and can also, due to positive feedback, influence the flame front oscillations dynamics. Accordingly, the study of such combined effects is of great current interest. The work is devoted to methane–air flames stability study, stabilized by the central body, under the external acoustic field, and different gravity conditions. It is shown that for laminar flames stability both the effect of acoustic field and gravity one is noticeable.

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Oxygen-free combustion—one of the latest ideas of V E Fortov

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A little more than ten years ago, Vladimir E Fortov suggested the possibility of initiating a detonation wave driven by the condensation energy of a supersaturated vapor. Several years later, when this idea was realized and the detonation wave of condensation was experimentally observed and studied, V E Fortov proposed to use this phenomenon for the development of a fundamentally new environmentally friendly energy cycle based on the use of the energy of carbon condensation formed during the pyrolysis of hydrocarbon fuels. In an interview in honor of his seventieth birthday, published in all media, Fortov said that when he resigns from the post of President of the Academy of Sciences and all other administrative posts, he would devote his research to oxygen-free combustion processes that allow obtaining energy from hydrocarbon fuels without emitting carbon dioxide. This lecture will present the stages and prospects for the development of this wonderful idea of V E Fortov, one of his main scientific interests in the last years.

Optical properties of soot synthesized in pyrolysis of ethylene and acetylene in shock tube reactor

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In this study, shock tube pyrolysis of 5% ethylene and 3% acetylene in argon was used to study the process of soot formation and properties of formed particles. The measurements of soot optical properties were performed at the temperatures behind reflected shock waves 1800–2000 K, corresponding to a maximum soot yield. The reaction time of the soot yield 1.5 ms within operation time of the shock tube was chosen due to at this time soot volume fraction reaches the plateau. The absolute value of the refractive index function of soot $E(m, 1064)$ at a wavelength 1064 nm and the ratio of the refractive index functions at two wavelengths of 532 nm and 1064 nm were measured by laser induced incandescence. The $E(m, 1064)$ was found to be 0.44 for acetylene soot and 0.35 for ethylene soot by comparing the measured peak temperature of laser heated soot with the calculated peak temperature obtained using laser induced-incandescence model. The ratio $E(m, 1064)/E(m, 532)$ was found to be 1.28 for acetylene and 0.8 for ethylene soot. The samples of soot nanoparticles were analyzed using high resolution transmission electron microscopy to determine the mean soot primary particle size and internal soot structure. The investigated optical and structural properties of shock tube pyrolysis soot were compared with the properties of acetylene and ethylene flame soot at corresponding mean soot particle sizes. A good correlation between the properties of pyrolysis and flame soot was obtained. This study was funded by the Russian Science Foundation, project 19-79-10204.

Influence of minor impurities of acetone on soot formation in acetylene shock wave pyrolysis

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Acetylene is an unique species that plays a key role in the formation of polyaromatic hydrocarons (PAH) and soot. However, many existing kinetic models can not satisfactorily describe the experimental results on the soot formation during the pyrolysis of acetylene behind shock waves. We analyzed the possibility that such a discrepancy was caused by a minor impurity of acetone inevitably contained in commercially available acetylene [1,2] which influence was previoulsy reported ambiguously [3,4]. Soot volume fraction time profiles in 3% C_2H_2 + Ar mixture at shock tube conditions $T = 1700$–2300 K and $P = 3.5$–4.5 bar was observed and modeled.

It was shown that in the presence of only 0.5 mol % acetone impurity in acetylene (i.e., 150 ppm in studied mixture) the values of the soot volume fraction observed in shock tube experiments at given time $\tau = 0.5$–1.5 ms can increase by several orders of magnitude, as fast acetone decomposition at elevated temepatures releases CH_3 radical providing pathways for propargyl C_3H_3 and benzene ring formation thus accelerating subsequent PAH and soot growth. The effect is exceptionally strong in considered case of realtively low pressures when the soot formation occurs slowly and soot yield at the end of shock tube working time amount to less than one percent.

The importance of controlled acetylene purification was emphasized.

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Experimental study of kinetics of C_3H_7I dissociation behind shock waves

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Iodine-containing halocarbons and halogenated hydrocarbons are widely used in various branches of the chemical industry, fire fighting and medicine. Therefore, scientific interest in such substances remains extremely high at the present time. In particular, the C_3H_7I molecule, due to the presence of the weakest bond between halogen and carbon atom (C–I bond), is the most suitable precursor for the alkyl radical C_3H_7. These radicals, as is known, are formed in significant quantities at the combustion and pyrolysis processes of normal alkanes, and without their correct prediction it is impossible to build physically based models of combustion of real hydrocarbon fuels. That is why this work is aimed at studying the kinetic properties of C_3H_7I dissociation. The reaction $C_3H_7I + Ar = C_3H_7 + I + Ar$ (1) has been studied at the temperatures 800–1200 K and pressures 3.5 ± 0.5 bar behind incident and reflected shock waves using the atomic resonance absorption spectroscopy (ARAS) technique on a resonant line of atomic iodine at 183.04 nm. The initial concentration of C_3H_7I in Ar was varied from 0.8 to 1.1 ppm. As a result, the first direct experimental data on the thermal unimolecular decomposition of n-C_3H_7I were obtained. Time profiles of iodine atom concentration were used to determine the temperature dependence of the rate constant of reaction (1) and its activation energy. Based on these data, the value of this rate constant was obtained in the two-parameter Arrhenius form, convenient for use in kinetic databases. It was found also, that under experimental conditions, the obtained values are close to the high-pressure limit.

Investigation of polycyclic aromatic hydrocarbons formation during shock wave pyrolysis of benzene and dimethyl ether mixtures

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Polycyclic aromatic hydrocarbons (PAHs) are mainly formed in incomplete combustion processes and generally considered as precursors for soot particles [1]. Precise measuring PAHs formation and growth is significant for better understanding and developing of soot formation kinetics [2]. In this work, laser-induced fluorescence (LIF) was used to detect PAHs formed during shock wave pyrolysis of benzene and dimethyl ether (DME) mixtures. To control the onset of the appearance of the condensed phase, the laser light extinction at 633 nm was registered. It was found, that PAHs LIF spectra shifts toward longer wavelengths with temperature and reaction time increasing. The addition of DME to benzene led to a shift in the PAHs LIF spectra towards shorter wavelengths relative the benzene mixture at the same initial temperature behind the shock wave. The modelling of kinetics of PAHs formation and growth was carried out using OpenSMOKE++ code [3] with a kinetic scheme [4]. The simulations have shown that DME presence leads to the formation of 5-membered aromatic ring (C_5H_5), $C_{10}H_{10}$, $C_{13}H_{10}$ as well as the emerging of alternative formation pathways C_9H_8 and $C_{10}H_8$. This work was supported by the Ministry of Science and Higher Education of the Russian Federation, agreement No. 075-15-2020-806.

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

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Propanol isomers (n-C_3H_7OH, i-C_3H_7OH) are promising applicants for the complete replacement of gasoline fuel. The main objective of this research was the experimental study of the interaction between isomers and oxygen at the high temperatures. The kinetics of reaction of biofuel with N_2O behind reflected shock waves is studied. The quantitative measurements of the time profiles of the concentration of oxygen atoms in the ground electronic state $O(^3P)$ were first carried out by the precisive method of atomic resonance absorption spectroscopy (ARAS) on a resonance vacuum-uv line of an oxygen atom at 130.5 nm. A study of the appearance and consumption of oxygen atoms during the reaction of propanol isomers with oxygen in mixtures 10 ppm N_2O + 1–10 ppm biofuel in Ar was performed. Along with the measurements, a detailed kinetic analysis was carried out using the Chemkin, consisting of a simulation of oxidation processes using current kinetic mechanisms and a corresponding sensitivity analysis of considered reactions. The data obtained in the course of a comprehensive study provide new valuable information on the features of the interaction of propanol isomers with oxygen at high temperatures, which will help both in verifying existing mechanisms and in creating new reliable kinetic schemes in a wide range of temperatures and pressures. The reported study was funded by the Russian Foundation for Basic Research (grant No. 20-58-12003).

Application of atomic resonance absorption spectroscopy on the oxygen atoms in chemical kinetics of high temperature reactions

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The formation of atomic oxygen occurs in most hydrocarbon and biofuel combustion processes. Various kinetic schemes make it possible to quantitatively calculate the appearance and consumption of atomic oxygen during combustion and pyrolysis processes. However, the verification of these models is based on accurate experimental data obtained under various conditions. The method of atomic resonance absorption spectroscopy (ARAS), as the gold standard of chemical kinetics, makes it possible to directly and reliably measure the concentration of atomic oxygen with the possible range of the measured concentration within 3×10^{11} to 10^{14} cm^3. As a result the rate constants of the reactions of various oxygen-containing compounds can be directly determined. The presented work shows the development of the use of O-ARAS method in shock tubes, starting from the dissociation reactions of simple molecules to the reactions of pyrolysis and combustion of complex alcohol compounds at 1200–2500 K and 2–4 bar. The possibilities of using high-power excimer lasers at a wavelength of 193 nm (500 mW per pulse) for photolysis of simple oxygen compounds with the immediate formation of atomic oxygen at the variable time after arrival of a reflected shock wave for studying combustion processes of various substances at 500–1200 K are discussed. The reported study was funded by the Russian Foundation for Basic Research (grant No. 20-58-12003).

Problem of South Pole–Aitken basin origin

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South Pole–Aitken (SPA) basin on the Moon is the largest impact structure in the entire Solar System. Its dimensions exceed 3000 km, and its depth reaches 9 km. There is no generally accepted explanation for the origin of this basin. The existing hypotheses suggest that the basin was formed about 4 billion years ago as a result of the fall of a very large cosmic body.
Based on the cumulative impact mechanism of the formation of large craters and sea basins on the Moon, Mars and Mercury, a hypothesis is substantiated, according to which we conclude the following.
The SPA basin arose not as a result of the impact of one large cosmic body, but as a result of multiple falls of high-speed galactic comets in periods of the last four bombardments of the Solar System by galactic comets.
The elliptical shape and a peculiar ring structure of the SPA basin are caused not only by the oblique incidence of galactic comets, but also by an increase in the angle of their incidence relative to the plane of the Moon's equator with each subsequent bombardment.
The time of the SPA basin formation should be considered Cenozoic, i.e., its age is 65 million years.

3. Equations of State for Matter

Equation of state for rhodium at high energy densities

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An equation of state for rhodium is proposed taking into account the effects of melting and evaporation. Calculations of thermodynamic characteristics and the phase boundaries of solid, liquid and gaseous Rh over a wide range of densities and temperatures are carried out. Comparison of calculated results with available experimental data and theoretical predictions at high energy densities is presented. Obtained multiphase equation of state for rhodium can be used effectively in numerical modeling of processes under conditions of intense pulsed influences on the material. This work is supported by the Russian Science Foundation (grant No. 19-19-00713).

Atomic number similarity law in individual electronic shells of all natural elements

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Experimental data on the electronic binding energies in atoms are analyzed using special reduced coordinates [1]. Application of the method to the analysis of K and L shells in many-electron atoms ($Z \geqslant 10$) [2] made it possible to describe experimental K, L_I, $L_{\rm II}$, $L_{\rm III}$ X-ray levels with an accuracy better than one percent and to control their reliability. The method has also shown its efficiency in the analysis of the internal and outer electron shells of lanthanides [3], detected patterns in the measured first ionization potentials of lanthanides and actinides [4].

In the present paper, we apply the method of studying the available experimental [5–7] and theoretical electronic binding energies [8] in all natural atoms of the periodic table ($1 \leqslant Z \leqslant 92$). Our goal is to show the general picture of the dependence of the measured binding energies in individual electron subshells on the atomic number, detect patterns and explain deviations from them and thus provide a way to recover missing or erroneous data.

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Volatile nature of liquid–liquid phase transition in dense hydrogen

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Liquid–liquid phase transition (LLPT) in dense hydrogen has been extensively investigated during the last decade. Theoretically the possibility of phase transition in non-ideal plasma has been predicted many years ago [1]. However up to now there is no direct experimental evidence of such a transition. LLPT in dense hydrogen at temperatures $T \lesssim 2000$ K has been discovered using first-principle simulations [2, 3]; in all predictions the phase boundary of such a transition has a negative slope. Very recent simulation papers [4, 5] claim that LLPT is situated at even lower temperatures (less than 1250 K) or even does not exist. In this presentation we analyze the properties of LLPT and its "volatile" character; in particular, we consider the miscibility of molecular and atomic (plasma) phases of hydrogen and the probability of phase boundary formation. The possibility of LLPT experimental observation in dense hydrogen is discussed. The work is supported by the Russian Science Foundation, grant No. 20-42-04421.

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Features of phase transitions in non-ideal plasmas

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The problem of both conventional (of van-der-Waals type) and non-standard phase transitions (PTs) in strongly nonideal plasma is discussed. This problem was one of the central for Vladimir Fortov, who passed away tragically few months ago. The first one is the very old and scandalous problem of great uncertainty in our knowledge for the high-temperature parameters and critical point location of gas-liquid phase coexistence in uranium and several "bad" metals. The second one is another old and scandalous problem of great uncertainty in our knowledge and in ability of correct theoretical description for the so-called non-congruent phase coexistence of fluid–fluid type in wide number of non-ideal plasma systems, e.g., plasma of metallic alloys, or that in high-temperature decomposition products for chemical mixtures and compounds like oxides, hydrides, nitrides, melting salts etc up to the exotic realization of non-congruence in dense nuclear matter and quark-hadron phase transformation. The last discussing topic is the problem of important but poorly recognized subclass of so-called entropic ("delocalization-driven") phase transitions in non-ideal plasmas of cosmic and terrestrial applications. The point there is that not only this type of (fluid–fluid) phase transitions themselves, but also a great accompanying region of anomalous thermodynamic properties (close to its critical point) are macroscopic manifestation for remarkable feature for entropic PTs—the multilayered structure of thermodynamic surfaces entropy, temperature and internal energy, $S(P,V)$, $U(P,V)$ and $T(P,V)$, within and around such phase transitions. Perspectives of experimental verification (both, real and numerical) for all mentioned above features concludes the discussion.

Thermodynamics of nonideal plasma in the SAHA model

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The central problem of the quasi-chemical description of the thermodynamics of a strongly coupled plasma (SCP), i.e., of the chemical plasma model (CPM) is the problem of correct and self-consistent accounting for the contribution of quantum bound states of many-electron complexes (atoms, molecules, atomic and molecular ions, etc) in a dense plasma environment. The idea of searching for a thermodynamically self-consistent combination of a quasi-classical description of the Coulomb non-ideality of "free" charges and a correct quantum-mechanical calculation of the contribution of substantially "constrained" bound states was initiated by V E Fortov in the 70s. This idea was the basis for the implementation of the so-called the "confined atom" model, where the total effect of plasma coupling was described in frames of the variational procedure and the concept of two "effective" potentials—external and internal (the calculation was carried out by the Hartree–Fock method). This model was applied to the thermodynamics of SCP of inert gases (neon, argon, xenon). Another example of a modern application of the CPM is the precise description of weakly non-ideal and weakly degenerate plasma of the Sun, where the data of long-term helioseismology observations provide extremely accurate knowledge of the effective hydrogen-helium plasma adiabatic exponent with small abundance of numerous elements. The report discusses the history and current state of both aspects of this problem.

Anomalies of spatial ions distribution in trap with different restraining potential

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Discontinuities in equilibrium spatial charge profiles of ions in non-uniform Coulomb systems is a common phenomenon in wide number of thermoelectrostatics problems. As we showed previously, such discontinuities are peculiar micro-level manifestation of phase transitions and intrinsic macro-level non-ideality elects in local equation of state (EOS), which should be used for description of non-ideal ionic subsystem in frames of local-density (or "pseudo fluid", or "jellium" etc) approximation. Special emphasis is made in present paper on the mentioned above non-ideality elects in non-uniform ionic subsystems, such as equilibrium charge profile in ionic traps with different "external potentials". Multiphase EOS for simplified ionic model of classical charged hard spheres on uniformly compressible electrostatic compensating background was constructed and several illustrative examples of discussed discontinuous ionic profiles were calculated.

Quantum-statistical calculations of equation of state of refractory metals

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We use the Hartree–Fock–Slater model with taking into account the band structure to calculate the thermal contribution of electrons to the equation of state of refractory metals (Ti, Cr, Nb, Mo, Re) in a wide range of densities (from 0.1 to 100 g/cm^3) and temperatures (from 0 to 100 keV). The calculated dependences are used to construct the Hugoniots of solid samples of these metals in the pressure range from 1 to 10^7 GPa. The comparison with the experimental data is given. This work is supportedby the Russian Science Foundation (grant No. 19-19-00713).

A wide-range multiphase equation of state for platinum

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This paper presents a semi-empirical wide-range equation of state (EOS) for platinum with account for melting, evaporation, and ionization. The equation is based on a wide spectrum of experimental and calculation data. Parameters for the EOS were adjusted using a genetic algorithm which proved to perform well for optimizations in big data processing. In the regions where no experimental data were available, we used results of first-principles and average-atom model calculations. The EOS was used to calculate the melting curve of platinum to pressures above 1 TPa, sound velocities along the Hugoniot curve, parameters of melting under shock compression, and parameters of the critical point. An improved model is proposed for the shear modulus in (V, T) coordinates and its variation along the shock adiabat is calculated.

Germanium and germanium–gold alloys under shock-wave loading

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The results of numerical experiments upon modeling of thermodynamic parameters such as value of pressure and compression of germanium and its alloys with gold are presented. The calculations were performed using the model TEC (thermodynamic equilibrium components). The model allows us to take into account the phase transition of germanium under shock-wave action. The interest in investigating of the compressibility for such materials is related both to the possibility of creating materials with the necessary properties and to the properties of the materials themselves. The results of calculations are compared with the known experimental results of different authors. The value of pressure and compression for shock wave loading of pure germanium and alloys with germanium as a component of various compositions are calculated.

Equation of state of fluid lead from exploding foils experiments

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The Mie–Grüneisen-type equation of state has been constructed for fluid lead based on results of the exploding foils experiments [1]. It is shown that the equation of state describes with sufficient accuracy thermodynamic properties of lead in the liquid and gaseous state as well as in the region of the metal-nonmetal transition occurring in the fluid on expansion. The nature of the transition is investigated based on its effect on thermodynamic functions and electrical resistivity.

The reported study was funded by the Russian Foundation for Basic Research and ROSATOM, project No. 20-21-00093.

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The sound speed measurements for liquid lead

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We are developing an experimental technique for the measurements the speed of sound in liquid metals at high temperatures (5–20 kK) and pressures (0.3–3.0 GPa), which are achieved in dynamic experiments [1]. Such experiments make it possible to measure the specific volume, pressure, specific enthalpy, and electrical conductivity of a sample for a quasi-static process, in which the volume, enthalpy, and pressure increase monotonically from normal values. To measure the speed of sound on the surface of the sample (a strip of foil placed between two plates of window material) an acoustic disturbance is generated using a laser pulse. The arrival of this disturbance on the opposite surface of the sample is recorded using a laser interferometer. The speed of sound is defined as the ratio of the thickness of the sample to the time interval during which the acoustic disturbance passes through it [2].

Experimental data on the dependence of the speed of sound in liquid lead on density and pressure are presented. The uncertainties of our measurements of the speed of sound are estimated.

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

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[2] Kondratyev A M and Rakhel A D 2020 *Non-ideal Plasma Physics Workshop, December 16–17 2020, Moscow, Russia*

Lateral effects in deformation of the window material plates in exploding foils experiments

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In the experiments [1], a metallic sample under study is sandwiched between two plates of the window material and heated by an electrical current pulse. During such an experiment the sample undergoes a nearly one-dimensional thermal expansion which results in compression of the window material plates. To estimate the errors of such experiments it is necessary to evaluate the effect of the lateral wave, which appears at the side surfaces of plates, on the thermal expansion of the sample. The problem of deformation of an elastic body in the form of a rectangular parallelepiped one of the surfaces of which is pushed by a flat piston, and the other surfaces are free is solved by using the theory of elasticity techniques.

The reported study was funded by the Russian Foundation for Basic Research and ROSATOM, project No. 20-21-00093.

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The thermal and "cold" ionization mechanism for conductivity of metal vapors in near-critical region

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The coexistence of vapor–liquid and dielectric–metal transitions has been discussed for many decades: it is not clear whether these are separate transitions or they coexist together. We proposed a new model [1] for calculating the metal vapor equation of state and conductivity in near-critical region. This method is based on the hypothesis of the existence of an electron jellium as an origin of the conduction band in metal-vapor gaseous phase. The jellium of the gaseous phase consists of the wave function tails of bound electrons lying outside the Wigner–Seitz cell (WS). The emergence of jellium leads to the appearance of cohesion—the quantum, collective binding energy of atoms. According to our hypothesis, the ion cores together with the jellium form a "gaseous metal" that exists at any density. In this work, the main properties of gaseous metal are considered. The temperature–density phase diagram shows the region of the "gaseous metal" state existence—the region where jellium electrons dominate thermally ionized electrons. The main properties of gaseous metal are discussed: the region of the gaseous metal existence near binodal; conductivity behavior at supercritical isotherms—the existence of minimum and asymptotics. The physical meaning of the conductivity "asymptotics" with density increase is the conductivity along the vapor–liquid coexistence curve. Our results are in good agreement with experimental and quantum molecular dynamics results [2, 3].

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Equation of state and the topology of hydrogen bonding networks in water at high temperatures and pressures

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Atomistic computer simulations of water using two different intermolecular potentials for H_2O were carried out for over 50 thermodynamic states covering a very wide range of conditions: $573 \leqslant T \leqslant 1273$ K; $0.02 \leqslant \rho \leqslant 1.67$ g/cm^3; $0.01 \leqslant P \leqslant 10$ GPa. Good agreement of the simulated thermodynamic and structural properties of water with available experimental data assures a reliable quantitative statistical analysis of intermolecular hydrogen bonding between H_2O molecules and the topology of the H-bonding networks formed under these conditions [1]. The effect of temperature on the energetic, geometric, and angular characteristics of H-bonding in water is much more profound than the effect of density along any supercritical isotherm over the entire density range from dilute gas-like (≈ 0.03 g/cm^3) to highly compressed liquid-like (≈ 1.5 g/cm^3) thermodynamic states. Both above and below the H-bonding network percolation threshold, the fractions of water molecules engaged in a certain specific number of H-bonds closely follow the universal binomial distributions as functions of the average number of H-bonds per one H_2O molecule in that state, $\langle n_{\mathrm{HB}} \rangle$, as predicted by a simple independent bond theory [2]. The universality of these distributions is preserved even when dynamic criteria of H-bonding lifetimes are additionally applied.

The research was supported by the HSE University Basic Research Program.

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Equations of state of the Mie–Grüneisen type as applied to problems of laser hardening of materials

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Strengthening of materials by means of exposure to laser radiation is one of the promising technologies in the field of interaction of laser radiation with matter. If ultrashort femtosecond laser pulses are used to strengthen metals, an almost isochorically heated region of increased pressure is created in the near-surface layer of the metal. A shock wave propagating from it deep into the metal changes the physical properties of the metal during its passage. Therefore, when calculating the dynamics of the target matter under the action of femtosecond laser pulses, especially in two-dimensional and three-dimensional cases, it is important to use the compact equation of state of matter, which describes well both the Hugoniot adiabat of the compressed substance and the Poisson adiabat of the expanding matter. As such an equation of state of matter, using the example of aluminum, we considered various versions of the Mie–Grüneisen equation of state with both constant and density-dependent Grüneisen coefficients using cold pressure and internal energy curves obtained as a result of calculations using density functional theory methods.

Thermophysical properties of the phonon subsystem of gold in the solid–liquid phase transition region: Atomistic modeling

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Studies of recent years have shown that gold nanoparticles demonstrate excellent imitation of the activity of biological enzymes. Pulsed laser ablation (PLA) is one of the common methods for generating nanoparticles. The generation of gold nanoparticles by PLA is carried out in a temperature range, in which the phase transitions play a decisive role. Studies of the kinetics and dynamics of phase transformations are carried out mainly by methods of mathematical modeling. PLA is accompanied by the phenomena of thermodynamic nonequilibrium, which leads to the need to take into account the characteristics of two subsystems: electronic and phonon. This report presents the results of atomistic modeling of the thermophysical properties of gold in the region of the melting–crystallization phase transition. The pressure dependencies of the specific heat of melting and equilibrium melting point, temperature dependencies of the density, linear size of the sample, coefficient of linear expansion, enthalpy, and heat capacity were determined. The obtained dependencies of the properties of gold are approximated by polynomials of low degrees. The results of comparing the obtained characteristics of this metal with experimental data show acceptable agreement. Numerical and graphical information about the obtained properties and the results of comparison with experimental data is presented.
The present work was supported by the Russian Science Foundation (project No. 18-11-00318).

Measurement of shock compressibility of silicon and softening of its Hugoniot curve at 200–500 GPa

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Previously, Hugoniot data on silicon in multi-megabar region was limited by Pavlovsky data (from 80 to 196 GPa), although well studied for pressures up to 60 GPa. However, theoretical calculations by Lomonosov (1996, semiempirical model) and Militzer (2016, quantum molecular dynamics) demonstrated significantly softer shock Hugoniot of Si, than Pavlovsky's experiment. In this work, experiments on shock compression of Si up to 510 GPa were performed to understand its Hugoniot. Mach-type explosive cumulative generators were used. Shock compressibility was determined by impedance matching with quartz reference. Two techniques were used to register the wave velocities in reference and sample. First is a fast optical detectors, registering the shock propagation in transparent reference and the exit of shock from opaque sample, a row of few detectors was necessary. Second is an infrared detector, possible to register the propagation of shock in both reference and sample due to transparency of silicon in infrared band. Experimental data, obtained at pressure 280–510 GPa, confirms the softening of Si Hugoniot, proposed by Lomonosov (1996) and Militzer (2016).

Sapphire melting curve at high pressure

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Sapphire is a rigid and transparent dielectric used in experiments at high pressures and temperatures. The transition of the substance from a crystalline to a liquid state is accompanied by a radical change in its properties. In particular, on both sides of the melting curve there are different densities, as well as specific values of internal energy, entropy and heat capacity. A change of the substance structure can lead to change of the mechanisms of electrical conductivity and heat transfer. The ability of the body to maintain shape disappears during melting, due to a change in the mechanism of resistance to shear stresses. Therefore, knowledge of the boundary between the liquid and solid states of a substance is incredibly important. At the same time, information about the melting curve of sapphire at high pressures is completely insufficient.

The calculation of melting curves is based on the Debye theory of heat capacity (in the case of metals, the contribution of the electronic subsystem to the heat capacity is also taken into account) and the Lindemann melting criterion. The shock adiabats determined in dynamic experiments and the thermophysical characteristics of the substance under normal conditions are used as basic experimental data. Mathematically, the problem is reduced to solving the Cauchy problem for a nonlinear system of ordinary differential equations. The system is solved numerically by the Runge–Kutta method. The comparison with the available calculated and experimental data, including the melting of sapphire in the shock wave, showed satisfactory agreement of the results.

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Equations of state of $CaCO_3$ phases based on the Helmholtz free energy

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The carbonates in the $CaCO_3$ system are important carbon carrier in the Earth's interior, transporting of carbon in the Earth's crust and mantle. Moreover, $CaCO_3$ phases are often found as inclusions in natural diamonds, being a source of information about their genesis. The $CaCO_3$ system was widely considered many authors, but the reliable thermodynamic description of $CaCO_3$ phases based on modern x-ray diffraction measurements is relevant. The thermodynamic properties of $CaCO_3$ phases can be calculated from their equations of state (EOS). The proposed equations of state of calcite, aragonite and postaragonite are based on the Helmholtz free energy by analogy with our previous studies for the Mg_2SiO_4 and $CaSiO_3$ systems [1–3]. The calculated equations of $CaCO_3$ phases contain group of fixed parameters and group of fitting parameters derived by least squares method in Excel worksheets. It is easy to calculate a full set of thermodynamic functions (entropy, enthalpy, Gibbs energy, etc) at given P–T parameters by the proposed approach.
The study was supported by the Russian Science Foundation (grant No. 19-77-00031).

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Structural features of the Seymchan meteorite substance after compressing by spherically converging shock waves

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Structural changes in the Seymchan meteoritic substance after the experiments on loading with spherically converging shock waves have been studied by optical and electron microscopy. It was noted that shock pressure and temperature increases from the outer part to the center of the loaded balls. In one experiment with shock-wave loading, it was possible to obtain varieties of textures with different degrees of shock and thermal metamorphism. These results prove that the shock wave loading experiment can be successfully applied in modeling space shocks and can be used to experimentally model processes at the small bodies of the solar system. The cooling rates of the melted zone of the shocked octahedral sample was estimated for the crystallization range.

The tensors of thermal deformation cyclotrimethylene trinitramine and hexanitrostilbene at atmospheric pressure

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The anisotropic thermal deformation of α-RDX (cyclotrimethylene trinitramine) and JD-X (hexanitrostilbene) in the range from 150 to 470 K for RDX and from 150 to 570 K for JD-X 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 axes and the characteristic surface of the tensors of thermal expansion are 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 for condensed α-RDX and JD-X materials.

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Description of isothermal compression of some molecular crystals

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The introduction of new methods to record fast processes, on the one hand, and development of computer engineering, on the other hand, have made numerical simulation one of the most efficient methods to study and analyze physical processes that allow one to obtain comprehensive and reliable information. All mathematical models of continuum mechanics are closed by equations of state (EOSs). It is shown that at present, despite numerous publications containing the results of experimental and theoretical studies, as well as publications on numerical simulation of thermophysical properties of materials, the challenges related to construction of EOSs still remain one of the central areas of research. When constructing theoretical models of EOSs for molecular crystals, it is assumed that pressure and internal energy can be split into two constituent parts: thermal and "cold" ones. The validity of the constructed EOSs should be checked by independent verification of the thermal and the "cold" constituents of pressure and internal energy using the known experimental data. The object of the present study is verification of the EOS derived by the example of molecular crystals of TATB, PETN, and RDX. The analysis of experimental data of isothermal compression of molecular crystals shows that the experimental and the calculated values are within the experimental error and are in good agreement. The proposed approach allows determining the pressure behavior under isothermal compression before running an experiment.

Effect of high pressure torsion at different temperatures on the structure-phase transformations in amorphous iron-based alloys

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The effects of the temperature (from 293 and 77 K) of deformation by high-pressure torsion (HPT) on the atomic structure of melt-quenched amorphous Fe83–xNiB17 alloys (x = 25, 29 and 33) and their crystallization thermal effect upon continuous heating have been analyzed by EXAFS in synchrotron radiation, transmission electron microscopy, and x-ray diffraction analysis. HPT at 293 K decreases the crystallization thermal effect, whereas HPT at 77 K increases it regardless of the alloy composition. The observed effect is caused by the reversibility of the structural transformations in the alloys upon variation in the deformation temperature. According to the results of the structure examination, HPT at 298 K leads to the formation of more ordered state (partially crystallized) of the initial amorphous alloys, while HPT at 77 K, on the contrary, stimulates the formation of even more disordered amorphous structure (by destruction of short-range order and an increase in the average values of the coordination numbers around the iron atoms in the first coordination sphere). This work was supported by the Russian Foundation for Basic Research (projects No. 20-32-70007) and the grant of President of the Russian Federation (No. MK-43.2020.2).

$V(P)$ equations of state of novel lanthanum and yttrium superhydrides

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Hydrides of metals are important materials for hydrogen and energy storage applications. High pressure is a very effective tool for the synthesis of new hydrogen-rich compounds, because it dramatically increases the Gibbs free energy of molecular hydrogen, stabilizing hydrides against decomposition into constituents.
Superhydrides, which are a class of recently discovered hydrogen-rich compounds with [H]/[M] > 4, demonstrate properties characteristic of atomic metallic hydrogen. Particularly, superconductivity with critical temperatures reaching 250 K in the La–H [1, 2] and 243 K in the Y–H [3, 4] systems was observed recently.
Presently, we discuss equations of state $V(P)$ of various lanthanum and yttrium superhydrides in the pressure ranges 120–163 and 160–255 GPa, respectively, studied with x-ray powder diffraction in diamond anvil cells at the 13-IDD beamline at GSECARS, Advanced Photon Source, Argonne National Laboratory.

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Room-temperature superconductivity in compressed polyhydrides

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The remarkable high-temperature superconducting behavior of H_3S (T_c = 200 K, [1]) and LaH_{10} (T_c = 250 K [2]) at about 150 GPa catalyzed the search for superconductivity in compressed ternary hydrides. The highest critical temperature of 288 K at 275 GPa has been found recently in the C–S–H system [3]. High-temperature superconductivity in these compounds is due to the formation of metallic hydrogen sublattice, which is obtained by pulsed laser heating of various elements with hydrogen at extremely high pressures achieved during compression on diamond anvils. In this report we will present new results of studies of high-pressure chemistry, magnetic and superconducting properties of YH_6, UH_7, ThH_{10}, $CeH_{9–10}$, PrH_9, NdH_9, EuH_9 and BaH_{12} binary and $(La,Y)H_{10}$ ternary polyhydrides discovered in the last 2 years by collaboration of IC RAS, LPI, Skoltech and Jilin University (China). Perspectives of design of light and magnetic sensors (SQIUDs) based on superhydrides synthesized in miniature diamond anvil cells will be discussed.

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Fluctuation mechanism of room superconductivity

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Spin–phonon–electron correlations in high-temperature superconductors (HTSCs) are considered in order to substantiate the possibility of increasing the critical temperature to 300 K and above. Criteria for the synthesis of new HTSC materials with a higher critical temperature are given. The values of the spectrum of spin waves are found, which resonantly interact with one of the three phonon modes, as a result of which coupled vibrations arise. The expression for the critical temperature, taking into account the spectra of spin-phonon vibrations, in the quasilinear approximation allows one to analyze its change with increasing pressure.

Anomalous behavior of acoustic high-frequency excitations along isobars

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Using molecular simulation, we studied the spectra of longitudinal and transverse excitations of water along two isobars. We have shown that the frequency of longitudinal excitations demonstrates strong temperature dependence at low temperatures and comes to saturation at high ones. The low temperature regime is in qualitative agreement with the experimental results reported in the literature. The high temperature regime has not been studied experimentally up to now.

The work is supported by the Council of the President of the Russian Federation for State Support of Young Scientists and Leading Scientific Schools, project No. MD-6103.2021.1.2.

Raman study of the solid solution of molecular hydrogen in the silica glass

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Solutions of molecular hydrogen and deuterium in silica glass with molar ratios $[H_2]/[SiO_2] = 0.6$ and $[D_2]/[SiO_2] = 0.63$ were synthesized at a hydrogen pressure of 7.5 GPa and $T = 250$ °C. A detailed study of these solutions by Raman spectroscopy revealed a significant effect of dissolved hydrogen and deuterium on the phonon spectrum of the silica glass matrix. The rotational and stretching modes of the hydrogen molecule appear in addition to the redistributed modes of silica glass. The same changes occur in the spectrum of silica glass deuteride, while the frequencies of the rotational and stretching modes of dissolved deuterium change in accordance with the isotopic effect in a diatomic molecule. The frequencies of the rotational and stretching modes of hydrogen are shifted, respectively, to the lower and higher frequencies in comparison with the frequencies in the gas phase. Such a strong mutual change in the phonon spectra of the silica matrix and hydrogen indicates the formation of hydrides of a new type, belonging to the class of inclusion compounds.

Hydrogen content and Raman spectra of the hydrogenated nanostructured amorphous silica

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The silica glass particles with diameter 5 nm can form nanostructures with the surface square about few hundred m^2/g. The hydrogenation of one of these nanostructured silica glass with surface square 326 m^2/g was carried out in a toroid-type high-pressure apparatus at $P = 5$ and 7.5 GPa and $T = 250$ °C for 24 hours and cooled to -196 °C to prevent hydrogen losses in the course of the subsequent pressure release. The hydrogen contents for the both samples, obtained by the hot extraction into a pre-evacuated volume, had the values $[H_2]/[SiO_2] = 0.55$ and 1 respectively. The Raman spectra of the both samples showed that dissolved hydrogen had the molecular form. However, the profiles and positions of the H_2 rotational and stretching lines on these Raman spectra denote on a significant amount of hydrogen molecules probably dissolved on the surface of SiO_2 particles.

Effect of boron on the structure of graphite formed at high pressure

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It has been experimentally established that high parameters (about 15–21 GPa and 1800–2500 °C) are required for the direct transition of graphite to diamond without the use of catalyst metals. However, if the synthesis of diamonds is carried out not from pure carbon, but, for example, from hydrocarbons, then the thermobaric conditions of such a transition decrease. Boron is one of the interesting and promising alloying additions to carbon. Despite a large number of studies on the mechanisms of the formation of graphite-like structures, many questions still remain unclear. In my report I will present the analysis of boron graphite microcrystals obtained under high pressure and temperature conditions. The experimentally obtained diffraction patterns of boron-doped graphite demonstrate a structure with a high degree of ordering, which improves with increasing boron concentration. At the same time, the substitution of boron for carbon atoms leads to significant local distortions in the graphene layers, and the intensity of D and D' peaks in the Raman spectra increases, which was noted earlier in [1]. The observed contradiction between the x-ray data and the Raman spectra is due to the fact that with an increase in the amount of boron in the graphene layer, the scattering of phonons by impurity atoms increases, while x-ray analysis gives only a general picture of the order. The refinement of the structure using x-ray data showed that the number of vacancies in graphene is higher than the amount of boron. Nevertheless, the answer to the question about the configurations of defect complexes of boron with vacancies requires further theoretical analysis. This work was supported by a grant from the Russian Science Foundation (No. 19-12-00111).

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Induced spin polarization in graphene via interaction with halogen doped MoS_2 and $MoSe_2$ monolayers

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Fabricating different heterostructures, it is possible to obtain new materials with unique properties [1,2]. The graphene/TMD (transition metal dichalcogenide) heterostructures seem to be particularly interesting. However, defects can significantly affect the properties of nanomaterials. By controlling the type, quantity, and location of defects in the material, it is possible to create completely new nanoelectronic devices.

The purpose of this work was to investigate the electronic properties of MoX_2/graphene heterostructures (X = S, Se) in which individual MoX_2 monolayers were doped by halogen atoms. The linear dependence of induced spin polarization on graphene near the Fermi energy on halogen periodic number was demonstrated. A possible way for detection of the arrangement of the dopants on the MoX_2 surface through STM measurements was presented. The obtained results open new prospects of the application of doped heterostructures in spintronics and optoelectronics.

The work was supported by the Russian Science Foundation (No. 18-73-10135).

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Structure of amorphous carbon experimentally quenched from the liquid state: Multiscale simulations

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The structure of amorphous carbon (a-C) experimentally quenched from the liquid state on a cold diamond substrate is numerically reproduced using a multiscale approach. At the macroscopic level, we solve the time-dependent heat conduction equation for experimental samples of actual size. As a result, we determine the distribution of the quenching rate, which varies with the distance from the substrate within 10^{14}–10^{12} K/s. At the microscopic level, we perform molecular dynamic simulation of the liquid carbon quenching using the obtained quenching rates. The density of the model a-C samples increases from 1.5 to 1.93 g/cm^3 with the decreasing of quenching rate from 10^{14} to 10^{12} K/s.

The main structural characteristics of the model a-C samples are studied in detail: the relative number of carbon atoms with different hybridization (sp^1, sp^2, sp^3), radial distribution function, angular distribution function, and the statistical analysis of rings. The structure of model a-C samples, depending on the quenching rate, varies from that of amorphous graphene to a highly porous material with a large number of sp^1 chains. We discuss the mechanisms underlying the strong effect of the quenching rate on the structure of a-C.

The present work is carried out as part of the fulfillment of the state assignment for conducting fundamental scientific research at the JIHT RAS (No. 075-00892-20-00) and related to the development of base principles for obtaining new materials and researching the problem of the behavior of metastable diamond under the influence of ultra-high temperatures.

Ab initio calculations of thermophysical properties of liquid metals in the vicinity of the liquid–gas coexistence curve

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The position of the binodal and critical point on a phase diagram of metals is necessary to know for the creation of adequate equations of state at densities below normal. Moreover, in the near-critical region of metals interesting phenomena have been predicted, in particular, the metal–non-metal transition and the cluster formation. Conventional steady-state or quasi steady-state experimental techniques are generally limited to below 2500 K, while results of the dynamic methods, in particular, on isentropic and isobaric expansion may be difficult to interpret because of the complexity of underlying physical phenomena. Moreover, an experimental measurement of critical parameters of metals is very difficult to carry out owing to extremely high temperatures (higher than 3000 K) and pressures (from kilobars to tens of kilobar). A theoretical calculation of near-critical metallic liquid causes significant difficulties because of the degeneration of the electronic subsystem and strong interaction. Unsurprisingly, that until recently there were no theoretical models able to consistently describe different types of dynamical experiments for metals in the vicinity of the liquid–gas coexistence curve. In this work, we are going to discuss our results of quantum molecular dynamics calculations of thermophysical properties and the estimation of critical parameters of W, Mo, U, and some other metals. The interpretation of available experimental data is also presented. This work has been supported by the Russian Science Foundation (grant No. 20-79-10398).

First-principles study of liquid zirconium by the method of quantum molecular dynamics

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Zirconium is one of the main structural materials for nuclear power plants. In this regard, accurate knowledge of the parameters at which the phase transition occurs is particular importance. However, its properties in the liquid phase are still only approximately known. This is due to the fact that experimental measurements by the electrostatic levitation method are limited to temperatures of 2.5–3 kK, and the complexity of measuring the volume of a liquid drop leads to a significant scatter in the density estimates. Either the interpretation of the experimental results by the method of pulsed heating of conductors is difficult due to the speed and complexity of the occurring physical phenomena.

Thus, it seems that at present the only available theoretical approach that can provide information of the thermophysical properties of a substance in the region of a hot expanded liquid is the first-principle method of quantum molecular dynamics (QMD) based on the electron density functional theory.

In this work, the selection of optimal parameters for subsequent modeling, QMD calculations of a detailed grid of isotherms and isochores for the solid and liquid phases and an estimate of the near-zero isobar of zirconium are carried out. Also, comparison with corresponding experimental data is performed.

Calculations were carried out in the Joint Institute for High Temperatures RAS under financial support of the Russian Science Foundation (grant No. 20-79-10398).

Ab initio calculations of transport and optical properties of Zr in the vicinity of melting

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Zirconium and its alloys are widelly applied in nuclear reactors as a cladding material for nuclear fuels because of its excellent resistance to corrosion, high melting temperature and a low neutron-capture cross-section.

In the present work, static and dynamic electrical conductivity for solid and liquid zirconium were calculated in the temperature range from 300 to 3000 K. The calculation is based on the first-principle method of quantum molecular dynamics (QMD) simulation, density functional theory and the Kubo–Greenwood formula [1]. The VASP package is used for QMD simulation. Then, using Kramers–Kronig transform, optical properties (normal emissivity, reflectivity and refraction index) are also calculated.

Calculations were perfomed with different technical parameters (total number of atoms in the QMD cell, **k**-points grid size, type of pseudopotentials) in order to show the convergence of the results. Comparison with the experimental data is presented.

This work has been supported by the Russian Science Foundation (grant No. 20-79-10398).

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Accuracy and limitations of some projector augmented wave pseudopotentials for metals at high pressures

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The method of projector augmented wave (PAW) pseudopotentials is widely used [1] to investigate properties of metals at extreme conditions, particularly high pressures. In this work, we study pseudopotentials presented in Vienna Ab initio Simulation Package [2] (VASP) in a wide range of pressures. Our research is dedicated to *ab initio* calculations of cold curves for several metals: Ag, Mo, Ti, Cu, Na, Mg, Zr, Rb, and Fe. Different crystal structures are considered for metals with polymorphic phase transitions. Additionally, the impact of the magnetic moment for Fe is studied. The limitations of pseudopotentials are analyzed by comparing with more accurate potentials. We also present the comparison of the calculated cold curves for different pseudopotentials with available diamond anvil cell experimental data. The work has been supported by the Russian Science Foundation (grant No. 20-79-10398).

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Calculation of electron transport properties of hot metallic plasma using semiclassic average atom model

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Interaction of intense laser pulses with metals usually leads to the formation of hot plasma, so that thermodynamic and transport properties of metals experience a dramatic change. To predict material response in such conditions, adequate wide-range models are required. Electron transport properties are usually defined in terms of Onsager theory [1]. Using the Boltzman equation [2] one can express the Onsager coefficients via the electron relaxation time and the transport cross section [2, 3]. The latter can be expressed using phase shifts of electron wave functions in an atomic potential [4]. In this study, we calculate the electric and heat conductivity for electrons in tin and aluminum plasma using a semiclassical average atom model: the bound electron states are evaluated using semiclassic wave functions, while Thomas–Fermi model is used to account for the free electrons. The resulting self-consistent potential is used to obtain the transport cross section and the Onsager coefficients. The calculated transport properties are then compared to available experimental data and more accurate theories. The work is supported by the Russian Science Foundation, grant No. 20-42-04421.

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Thermodynamic properties of diatomic gases from quantum chemistry

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Thermodynamic databases are at the heart of different engineering challenges, such as designing rocket engines and new materials with special properties, chemical engineering, metallurgy, mining, waste processing, etc. Updating these databases can be performed using both new experimental results and contemporary quantum chemistry methods. The computational methods become more essential for the molecules that cannot be studied experimentally due to their short living times and extreme conditions. A particular example of such system is the formation of argon diatomic molecules in plasma at elevated temperatures. Previously, electronic states were studied and thermodynamic functions were calculated for a number of such compounds [1–4]. However, in these studies we relied on quantum chemistry results of other authors. This paper presents our new approach for calculation the thermodynamic functions of positively charged argon nitride (ArN^+) using ab initio quantum chemical calculations. For this molecule, the temperature dependences of the main thermodynamic functions were obtained and the error estimates were given.

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Semimetallic and metallic states of crystalline molecular hydrogen

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The transition of molecular crystalline hydrogen from the semiconducting state to the semimetallic and metallic states has been discovered upon compression in the pressure range of 302–626 GPa along the 100 K isotherm.
At pressures below 361 GPa, the molecular crystal with the C2/c structure is a semiconductor with an indirect gap. Upon further compression, the indirect gap between the conduction and valence bands closes. In this case, the direct gap remains open. Thus, in the pressure range 361–527 GPa, the valence band is partially unoccupied, and the conduction band is partially filled, which indicates the semi-metallic nature of the conductivity. Moreover, the formation of a semi-metallic state is accompanied by a sharp increase in electrical conductivity in a narrow pressure range from 361 to 389 GPa, which is in a good agreement with the experimental data.
When compressed to pressures above 544 GPa, the structure changes from monoclinic C2/c to orthorhombic Cmca, accompanied by a sharp decrease (by more than two orders of magnitude) in the value of the direct gap, which is an indication of the metallic nature of the conductivity of the resulting structure. The resulting metallic state is metastable and exists up to a pressure of 626 GPa.
The work is prepared within the framework of the HSE University Basic Research Program.

Investigation of new metastable crystal structures of solid molecular hydrogen

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Under high enough pressures, hydrogen should form a crystal lattice. It is predicted that this hydrogen phase is a high-temperature superconductor. Three new metastable crystal structures have recently been predicted [2]. This information is sufficient to accurately calculate the superconducting transition temperature. Aiming that, we need to find the phonon spectra of these structures. In this work, we investigate the change in the structure and symmetry of hydrogen depending on pressure. We also obtain a cold isotherm for the newly predicted structures. The parameters of the calculation of the phonon spectrum of metastable solid molecular hydrogen are selected within the framework of the density functional perturbation theory method, which is implemented in the PHONon Quantum ESPRESSO software package. We use the Perdew–Burke–Ernzerhof exchange-correlation functional and a projector augmented wave pseudopotential from the Quantum ESPRESSO software package. We also select the parameters for calculating the dynamic matrix: the value of the basis of plane waves [5] and the grid of integration in the Brillouin zone. Current work shows that the new structure of hydrogen is quite stable due to symmetry, but the size of the unit cells can vary significantly. It also turns out that one cannot rely on the standard values of the listed parameters. On the basis of the results obtained, we discuss the applicability of the method used for calculating the transition temperature to the superconducting state.

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Anharmonic lattice dynamics calculations of crystalline hydrogen

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According to the theoretical predictions, crystalline hydrogen should have a number of unique properties [1]. In the present work, phonon calculations are performed for the phases of crystalline hydrogen that are stable at 100 K [2]. In addition to the conventional scheme based on the harmonic approximation, temperature and anharmonic effects are also considered. For calculation of harmonic force constants, finite displacement method is used. Forces are calculated in the VASP package [3–6]. Temperature and anharmonic effects are considered by using the model [7] as implemented in the DynaPhoPy package [8]. Ab-initio molecular dynamics simulations are performed in the VASP package. Corresponding force constants are used to calculate phonon spectra in the PhonoPy package [9]. Anharmonic and temperature effects lead to stabilization of the phases.

The work has been funded by the Russian Science Foundation (grant No. 18-19-00734).

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Equations of state and elasticity of brucite and portlandite at high temperatures and pressures from classical atomistic simulations

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Brucite, $Mg(OH)_2$, and portlandite, $Ca(OH)_2$, have a similar hexagonal layered crystal structure that is held together by hydrogen bonding between the hydroxyl groups of the opposing layers. The thermodynamic and elastic properties of such minerals at high temperatures and pressures are of great importance for fundamental geochemistry and geophysics. The ClayFF force field [1] has been originally developed for classical atomistic computer simulations of clays and their hydrated interfaces under ambient conditions. Here we are using its new recent modification, ClayFF-MOH [2], more accurately accounting for the bending of Mg–O–H and Ca–O–H angles in the crystal structures, in order to test the applicability of this model at high temperatures and pressures well beyond the range of the original ClayFF implementation. The P–T dependencies of brucite and portlandite crystallographic parameters, the compressibility of their crystal lattices, the coefficients of thermal expansion, and the vibrational spectra are calculated in a series of classical molecular dynamics simulations using the ClayFF-MOH model. The research was supported by the HSE University Basic Research Program and used the NRU HSE supercomputer.

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Consideration of a heterogeneous medium taking into account the microstructure

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Issues related to taking into account the microstructure (geometry and physical characteristics of phases) of a heterogeneous medium, its influence on the behavior of the entire system and its changes present significant difficulties. Based on the use of continual approaches to describe heterogeneous media [1], a mathematical model was built that takes into account the elastic properties of a heterogeneous system and displays the microstructure of a heterogeneous system and its change under the influence of loads. The microstructure is taken into account by introducing a non-local operator in methods based on the Green's function, which with the subsequent convolution of the Green's function with the correlation function of the structure geometry allows one to take into account the microstructure of the system in a more general form. The study is carried out for a heterogeneous material [2] obtained by the method of cold gas-dynamic spraying with subsequent laser treatment. In this regard, the presented in the model information on the evolution of the microstructure takes into account the dissolution process and the occurrence of a chemical reaction (the model takes into account the mechanism of a decrease in the size of boron carbide B4C particles). The model contains information about a significant change in the properties of the structure. The reported study was funded by the Russian Foundation for Basic Research according to the research project No. 20-31-70001.

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Classification of particle interaction potentials based on physical parameters of particle system

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In systems with different potential of particles interaction, physical quantities can differ [1]. The main factor of the interaction can be the gravitational potential, the Lennard-Jones potential, its modifications etc. Examples of such systems are different materials or the composition of different space systems such as gas stars. In this work, I investigated the sensitivity of the transfer coefficients and other physical quantities to a change in the interaction potential, both in the form of a change in the parameters of the potential, and in the form of a functional change. The question of the "proximity" of potentials in the sense of their influence on the macroparameters of systems is investigated. Calculations are carried out in the LAMMPS software package. On the basis of the studied characteristics of the systems, I made a classification of the potentials of different functional behavior. For classification is done by using machine learning methods with small databases, assuming a priori distribution. Current work shows that, despite the functional difference, different potentials can realize the same macroparameters in the system. It turns out that this phenomenon is observed in real life and corresponding examples are given. On the basis of the results obtained, the I discussed the question about what can be expected from structures that are (so far) guessed in computational physics but have not yet been obtained experimentally.

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Experimental study of thermal expansion of refractory metals near its melting point

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Millisecond electrical pulse heating is a prominent method for studying the thermophysical properties of refractory metals at high temperatures. Meanwhile, some of the properties of such materials, in particular, iridium and vanadium, are still insufficiently investigated at this melting temperature region.

This work contains an experimental investigation of the temperature dependences of the thermophysical properties of iridium and vanadium at high temperatures and in the melting region by the method of pulse electrical heating.

Using this method, an experimental investigation of the thermal expansion coefficient, electrical resistivity and emission spectra at premelting region of iridium have been carried out. The obtained temperature dependences of the thermophysical properties of iridium and vanadium are of interest, in particular, for constructing wide-range equations of state, as well as for use in new high-temperature technology.

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Influence of the spectral interval choice on the temperature determination accuracy by multiwave thermometry methods

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Using model examples, the analysis of the instrumental accuracy of determining the model temperatures from data on the measurement of radiance temperatures for two and three experimental points is carried out, when neither the thermodynamic temperature nor the emissivity of the sighting site are known. An estimate of the instrumental accuracy of determining the desired temperature depending on the choice of the spectral window in the thermal radiation spectrum is given. It is shown that moving the spectral window to the long-wavelength region of the thermal radiation spectrum can worsen the instrumental accuracy of the desired temperature by several times.
For two wavelengths this problem was briefly discussed in [1].

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The statistics of clusters in the system of intersecting spheres randomly distributed in space

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The new type of distribution function of particles over the clusters have recently been introduced previously [1]. The distribution belongs to a system of identical intersecting spheres with radii R, the centers of which are uniformly distributed in space. Consideration is based on the concept of the rank number of clusters, where the rank is assigned to clusters according to the cluster sizes. The distribution function has some standard form, which does not depend on boundary conditions and is valid for infinite medium. The shape of the distribution function depends only on one parameter. It is the ratio $a = R/l_0$, where $l_0 = 0.554n^{-1/3}$ is the mean distance between "particles" (i.e., centers of spheres), which are assumed to be randomly distributed over the whole volume V, and the particle density, $n = N_0/V$, N_0 is the number of "particles" in the system. We study the properties of the standard distribution in detail and its applications to some realistic physical situations, which are close to the conditions of the gas condensation to liquid.

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Hydrodynamical model for capillary oscillations of sessile drop

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The exact solution of capillary oscillation problem for free and sessile droplets forms the base for the liquids surface tension determination by the dynamic methods [1–3]. Such analytical solution for free spherical nucleus have been used to extract the viscosity of hadronic matter from nuclei data [4]. In this work, the capillary oscillations of a sessile droplet with fixed or mobile contact line is considered. Within the framework of the polynomial expansion method for surface displacements from the equilibrium position, a system of equations were constructed and solved for normal oscillation modes. For the fixed contact line, a comparison with the solution of the integro-differential equation obtained in work [5] was made.
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Wetting by gallium microdroplets and its eutectic Ga–In and Ga–Sn alloys of highly oriented graphite intercalated by alkali metal atoms

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The effect of two-zone graphite intercalation and laser doping with potassium atoms on the contact angle of wetting by gallium microdrops has been investigated. It has been shown that intercalation of graphite with potassium leads to the effect of wetting the initially non-wettable basal plane of graphite. Scanning electron microscopy shows the effect of decreasing the wetting angle from 85° to 45° while reducing the size of gallium droplets from 5.4 to 1.43 μm. The experimentally found values of interfacial energies are compared with the Thomas–Fermi–Dirac statistical model [1].
This work was supported by grant from the Russian Foundation for Basic Research (No. 18-02-01042).

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The capillary vibrations method to study the interfacial tension of eutectic gallium alloys at the interface with vacuum and electrolyte solution

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A new technique for measuring the dynamic and geometric characteristics of strongly curved interfaces has been developed and implemented. The method based on capillary vibrations of a microliter droplet "hanging" at the end of a capillary or "lying" on a substrate in a gaseous medium, vacuum or liquid. To study the capillary properties of low-melting alloys, an experimental setup with signs of patentability has been designed and manufactured. The surface tension of microliter droplets of gallium and its eutectic alloys with tin and indium in vacuum and inert medium, as well as at the interface with aqueous solutions of hydrochloric acid and sodium hydroxide, has been measured for the first time by the method based on measuring the spectrum of capillary oscillations [1].
This work was supported by grant from the Russian Foundation for Basic Research (No. 18-02-01042).

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Comparison of two equations of state near the liquid–vapor transition region

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This work is devoted to the description of the thermodynamic properties of matter near the region of the liquid–vapor phase transition. The calculations of the boundaries of the liquid–vapor phase equilibrium, as well as the boundaries of stability of metastable states of the liquid and gas phases were carried out using two models of the equations of state: Van der Waals and Likalter. The calculation results are compared with the available experimental data on the temperature dependence of the density of liquid and saturated vapor for mercury and cesium.

Similarity of properties and similarity criteria

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The similarity of the properties of substances manifested in the one-parameter law of the corresponding states. The most known parameters are the critical compressibility factor Z_c and the Pitzer acentric factor. The subject of our analysis is two forms of the similarity criterion A by L P Filippov. The form chosen at the thermodynamic level is clearly related to the van der Waals equation of state (EOS). This makes it possible to connect the results obtained by us for a new one-parameter family of EOS, including many van der Waals type EOS. At the molecular level, the A capabilities appear after deciphering its connection with the shell molecule fundamental characteristic—its "rigidity". It calculates as a function of the atoms number in the molecule and the atomic shells overlapping degree. By determining the nature of the interaction, rigidity creates the intermolecular curves features into the singular points form. These features are projected into the thermodynamic surface features, including the critical parameters. In the empirically found expression, which relates the critical volume to the molecule size, L P Filippov "groped" for another fundamental point. The point fixes the inflection of the intermolecular force curve, which manifests in the Guldberg ratio. It concludes that it is precisely the "rigidity" that reflects the nuclear-electronic structure of a real molecule and ensures the similarity of interactions and properties. The work dedicates to the 95^{th} anniversary of L P Filippov.

Features of the description of the coexistence curve of pure substances in the range from triple to critical point

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The question of modeling the coexistence curve of pure substances on the basis of various models of the average diameter and order parameter is considered. In particular, the Yang–Yang model is considered, which has found application in describing the saturation line of individual substances (argon, C_6F_6 and SF_6, ethane, etc. [1]) and metals [2] in the temperature range from the triple point to the critical point. The proposed approach is based on the modified Clapeyron–Clausius equation:

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

Here ρ^- is the density on the vapor branch of the coexistence curve; p_s is the saturated pressure; T is the temperature; $r^* = r^*(T)$ is the function that is related to the heat of vaporization by the dependence

$$r = r^*\left(1 - \frac{\rho^-}{\rho^+}\right), \tag{2}$$

where ρ^+ is the density on the liquid branch of the coexistence curve.

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Comparative analysis of some models describing densities of the liquid and the gas at the saturation line for SF_6

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This report considers some problems, which are connected with the behavior of the gas density (ρ_g) and the liquid density (ρ_l) at the saturation line of SF_6. We pay an attention to some thermodynamic models, $\rho_l(\tau)$, $\rho_g(\tau)$, which have a scaling form, here $\tau = (T_c - T)/T_c$ is the relative temperature, T_c is the critical temperature. There is an Anisimov model between these models. The model is valid at relative temperatures, $0 < \tau < 0.02$, and includes scaling components with indices, α, β, 2β, ... Another model is developed in the work; the model is referred to as a combined scaling model and works up to $\tau \approx 0.1$ for SF_6. We have investigated one more problem: to evaluate (ρ_l, ρ_g, τ) data of SF_6 accordingly to experimental (h, τ) data [1] in the interval, $\tau = 10^{-2}$ to 10^{-6}, here h is the position of the meniscus. The last separates the liquid and gas phases of a sample. This sample of a substance is placed in a horizontal cylinder. It is shown that the function, $y(\tau) = 2h/d$, can take values in the range, $y = -0.04$ to 0.03, if τ decreases in the interval, $\tau = 10^{-2}$ to 10^{-6}. We have solved a number of tasks, including: (i) to investigate $y(\tau)$ theoretically, (ii) to evaluate (ρ_l, ρ_g, τ) data of SF_6 accordingly to experimental (y, τ) data [1], (iii) to build a combined model, which let us describe the coexisting densities (ρ_l, ρ_g) at temperatures, $0 < \tau < 0.1$.

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Modeling the composition of the Earth's core

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The outer core of the Earth is liquid, so the equation of state (EOS) of a condensed medium is sufficient to model its characteristics and composition.

The main problem in constructing the EOS is to find the interaction potential of the particles of the medium. The problem is solved either empirically or from "first principles". The shock wave data, which can be obtained in the entire range of interest for the existence of a condensed medium, are most adequate to the problem posed.

In our work, the connection between the potential compression curve and the shock compression curve of the medium, necessary for constructing the EOS, was found from experimental data, modeling by molecular dynamics methods and qualitative substantiation.

The semiempirical EOS of a condensed medium obtained by us is used to select a light addition to the iron-nickel core of the Earth in such a way as to explain its characteristics: pressure, density, temperature and speed of seismic waves in the core.

It was found that the main necessary additive can be carbon, both in free form and in the composition of simple chemical compounds.

The results of the calculations are also compared with the known data for iron and carbon, which are important elements in the physics of the Earth and in applications.

4. Methods of Mathematical Modeling

Comparative estimation of the properties of liquid metals at high temperatures and pressures using the methods of classical and ab initio molecular dynamics

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One of the foreground tasks of computer simulation is the prediction of metal properties at high temperatures and pressures, for example, under shock compression conditions. Recently the embedded atom model (EAM) was applied to describe highly compressed states, as a result were calculated multiparticle interatomic potentials of metals. Another method for calculating properties under shock compression is the ab initio quantum mechanical method. It allows the properties calculation without attracting any model approximations but it requires a lot of power and is really time consumable. To estimate the forecasting power of both methods, we compared the data obtained for the same states under conditions of shock compression for four liquid metals Na (4000 K), Bi (10 000 K), Ni (4450 K) and Fe (6000 K). Both methods gave similar results for the coefficient of self-diffusion and the functions of the pair distribution of atoms but the pressure difference can reach up to 30%.
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Nanobubbles diffusion in metals: Theory and atomistic modelling

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Diffusion of gas bubbles in nuclear materials plays a significant role in their mechanical properties and in fission gas release processes from fuels. The presence of stable facets of nanobubbles in crystal lattice can significantly affect their diffusion coefficient [1], but the existing theory of this phenomenon is too general and cannot take into account atomistic structure of nanobubbles in a given material. Such a theory for the mechanisms of bubble motion in crystals can be extended and developed using methods of atomistic modelling [2]. In this work, we consider the movement of bubbles in the several bcc and fcc metals and report the analysis of possible mechanisms of diffusion for empty bubbles and for gas-filled bubbles [3, 4].

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Mechanisms of overpressurized xenon nanobubbles diffusion in UO_2

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The diffusion of gas bubbles in nuclear fuels is an important topic for radiation materials science. The greatest attention is focused on the diffusion of xenon bubbles in uranium dioxide, as the most common nuclear fuel. The gas pressure is considered to be the key factor suppressing diffusion of nano-size bubbles [1, 2]. Verma estimates the diffusion coefficient of a bubble with a radius of 0.4–1 nm at a temperature of 1873 K: the magnitude of suppression is about 17 orders [3]. However this estimation lies far from experimental data [4]. In the present work, molecular dynamics modeling of xenon bubbles with a radius of 6–10 Å is carried out. Simulation made it possible to consider the kinetics of the diffusion process.

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The formation energies of magnetite vacancies within the density functional theory +U

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Ab-initio calculation of the magnetite point defects properties is a computational physics problem that is relevant for many magnetite applications nowadays. Magnetite is a magnetic iron oxide with strong electronic correlations. The calculation requires a method that able to take it into account.

The properties of isolated point defects of magnetite obtained in previous works are very contradictory. Indeed, the formation energies of A- and B-vacancies obtained within density functional theory (DFT) +U are 3.45 and 2.30 eV [1], respectively, while without correction for the same defects, the values are 2.69 and 0.83 eV [2]. Analysis of the literature data shows that the reason for such contradictions may lie in the high sensitivity of the DFT+U cubic phase magnetite model to the calculation method [1, 3, 4].

The report discusses a set of assumptions (the effective correction term U_{eff}, the size of the supercell, initial approximations to the wave functions and electron density, geometry optimization parameters), which gives adequate values of the formation energies of magnetite cubic phase vacancies within DFT+U. The results are compared with the results of calculations without the Hubbard correction.

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Defect formation energies in FeO: A comparison of molecular statics and molecular dynamics

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Point defects affect various properties of crystals, for example, electrical conductivity, self-diffusion processes, and phase transition parameters depend on their concentration and mobility. The concentration of defects can be obtained directly from molecular dynamic calculation [1], but this method requires huge computational resources. At the same time concentration of point defects can be described in terms of the free energy of defect formation. Using the chemical potential, the concentration can be obtained from static calculations. However, the use of the chemical potential in multicomponent crystals raises the question of the choice of reference state. In this work, we use iron oxide FeO with a Tersoff potential [2] as a model of a two-component crystal, for it we obtain and compare the defect energies from both methods.

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Molecular-dynamical model of crystalline lysozyme

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Comprehensive studies of proteins are essential for a variety of challenges faced by humanity nowadays. Modern techniques of decoding protein sequences are now mostly automated and do not require many resources. However, the three-dimensional (3D) structure of a protein is important in addition to its sequence to deeply understand its functions. The x-ray method is considered to be the classical approach to obtaining 3D protein structures. Unfortunately, the crystallization of a protein is needed for it. This can be an issue because of peculiar experimental conditions often necessary for crystallization. Moreover, it is sometimes impossible to crystallize a protein due to its specificuty. Artificial mutations can help, however, they complicate the process as many variations of a protein need to be crystallized. Molecular simulations are used extensively to search for mutations fostering protein crystallization. Furthermore, a molecular-dynamical (MD) model of a crystalline protein can be used to interpret experimental data. An MD model of crystalline lysozyme is created in this work. Neutralization techniques and effects of pH are analyzed [1,2]. The temperature dependence of equilibrium humidity is calculated. Convergence in multiple macroscopic measures is proven. Water mobility is studied. Spatial distribution of mobile water molecules is obtained.

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Exciton dissociation in warm dense molecular hydrogen

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The transition from the molecular to the atomic state in warm dense fluid hydrogen has been the subject of active scientific research in the last few decades. The use of various experimental techniques has not yet led to reliable consistent results. Despite numerous attempts, theoretical methods have not yet been able to explain the existing discrepancies in the experimental data and the microscopic nature of the mechanism of transition of the hydrogen fluid to the conducting state. In [1] the importance of taking into account non-equilibrium non-adiabatic processes in the analysis of the mechanisms of the transition under consideration was shown. This work presents the results of calculations of the properties of exciton states formed as a result of spontaneous vibronic excitations. It is shown that the dissociation of such excitons at high temperatures can explain the experimentally detectable characteristics of the transition under consideration.

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Polymorphic transformations and melting of ice XVII: Molecular dynamics modeling

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Depending on temperature and pressure water molecules in the solid state may give rise to more than 17 different forms of ices. In 2016 del Rosso *et al* [1,2] were able to empty the Co clathrate of hydrogen and to identify the obtained structure as a new form of ice, ice XVII. Recently del Rosso *et al* [3] have described a new method to obtain pure cubic ice Ic in large quantities from ice XVII.
It is known that the TIP4P/Ice model used in this work describes different characteristics of the solid phase of water with high precision. In this work, the transition of ice XVII into cubic ice Ic was obtained using molecular dynamics methods. The mechanism of such a transition was shown. The latent heat of the phase transition and the rate of formation of cubic ice Ic have been calculated. The probability of the formation of cubic (Ic) or hexagonal (Ih) ices depending on the temperature was obtained. Also, different characteristics of ice XVII were determined by molecular dynamics methods and compared with experimental data.

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Calculation of the elastic properties of amorphous ice: Molecular dynamic simulation

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In contrast to ordinary first-order transitions, the kinetics of transformations from crystalline to amorphous and amorphous to amorphous state is much less understood. Lattice instability is supposed to be the mechanism triggering solid-state amorphization (SSA). Cooperative vibration soft modes may be responsible for coordination changes in amorphous phases the displacive mechanism. For a microscopic understanding of how such transformations take place in crystalline and amorphous ices, the molecular dynamics (MD) method is an effective theoretical tool. In this work, the model of ice TIP4P/Ice is considered, amorphous ice of high (HDA) and low (LDA) density is obtained. The transformation of one amorphous form into another is considered. Calculation of elastic properties of amorphous ice has been carried out, the result is compared with experiment [1]. System modeling and calculations are implemented using the LAMMPS package.

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Molecular dynamics modeling of protein diffusion in an aqueous solution

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The movement of proteins in the cell cytoplasm plays an important role in the functioning of cells of living organisms. A quantitative characteristic of such processes is the diffusion coefficient. In this paper, the simplest model is considered for the quantitative description of the diffusion of a small lysozyme protein in an aqueous solution. At the first stage, the protein is released for relaxation in water, and then attempts are made to calculate the diffusion coefficient of this protein in water in various ways.
The first method is to use the Einstein relation

$$D = \mu k_b T,$$

where D is the diffusion coefficient, μ is the protein mobility, and k_b is the Boltzmann constant, T is the absolute temperature of the system.
The second method is using the Stokes–Einstein formula

$$D = \frac{k_b T}{6\pi\eta r}$$

to estimate the diffusion coefficient. Here η is the viscosity coefficient of water at the desired temperature, r is the gyration radius of the protein (the characteristic size of the protein). The formula has this form, because in the work the whole protein moves translationally, possible rotations are not investigated.

Transport processes in aqueous sucrose solutions

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Mono- and polysaccharides are widespread in nature, but at the same time they are of great industrial importance. Of particular interest are membranes based on cellulose esters, which are used in the desalination of seawater or its purification from high-molecular impurities and heavy metal impurities. Cellulose ester-based membranes may also be promising considered as separation membranes in electrochemical current sources such as Red/Ox elements. This results in the importance of studying the properties of aqueous solutions of mono- and polysaccharides, as well as the interaction of insoluble polysaccharides with water. Some of the defining characteristics are the transport properties: diffusion and viscosity. To study transport processes in solution, we can use the method of molecular dynamics. The accuracy and reliability of its results is determined by how well the used force fields reproduce the interactions of the studied molecules with each other and with water molecules. In this paper, the model of an aqueous sucrose solution is studied and investigated for the dependence of the viscosity and diffusion coefficients on temperature. The viscosity coefficient is determined by the Green–Kubo method, and the diffusion coefficient is derived using Einstein–Smoluchowski relation. In addition, the equilibrium density of the system in wide temperature range is calculated.

Water solution of 1,4-dioxane: Molecular dynamics method

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We investigate physical properties of water solution of 1,4-dioxane using molecular dynamics and two force fields to describe dioxane molecules: Smith's model [1] and modified OPLS-AA [2]. The obtained results may be useful for simulations of polymer membranes in Red/Ox flow batteries. One of the features of the Smith's force field is an additional term in the formula of non-bonded interactions, which explicitly describes hydrogen bonds in solution. Water interactions are represented by three versions of TIP4P model developed in 1983, 2004 and 2005. The solution density, enthalpy of solvation and viscosity are calculated over the whole range of dioxane concentrations. A combination of Green–Kubo formula with double exponential method [3] is applied to calculate viscosities. Results of the calculations are compared to the experimental data [4, 5]. We discover that the Smith's force field is able to reproduce the experiment accurately whereas the OPLS-AA model demonstrates significant discrepancies with the experimental data. These discrepancies imply that the dioxane affinity to water is excessive in this model. The structural analysis of the solution confirms this implication.

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Solvation of divalent ions in organic solvents

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Molecular dynamics simulation of divalent ion solvation in organic solvents is carried out. Various liquids are considered as solvents. It is shown that solvent molecules are bound to ions via oxygen atoms. As a consequence ion coordination number is weakly dependent on the solvent. A theoretical model of the ion solvation in organic solvent is developed and tested. It is in a good agreement with the molecular dynamics results.
This work is an output of a research project implemented as part of the Basic Research Program at the National Research University Higher School of Economics (HSE University).

Transport properties of confined liquid hydrocarbons in slit pores

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The transport properties of liquid hydrocarbons in slit pores with mineral walls are studied using non-equilibrium molecular dynamics methods. Hydrocarbons and walls are simulated with the OPLS2017 [1] and ClayFF [2] force fields, respectively, and pore widths from 2 to 7 nm are considered.
Non-equilibrium molecular dynamics simulations are performed for Couette and Poiseuille flows. For Couette flow, the Müller–Plathe approach [3] is used. To simulate a constant pressure gradient for Poiseuille flow, equal forces are applied to each molecule of the fluid. From the velocity profiles for flows, shear viscosity of the fluid and fluid-wall slip length are calculated. The viscosity–density dependencies for various pore widths are constructed by taking the Voronoi tessellation of the system and considering the total number of Voronoi cells centered on molecules of fluid as the fluid volume.
The simulations show that the viscosity–density dependence of the fluid is practically independent of the distance between pore walls, even for the smallest widths (2–3 nm) The slip length is of the order of the intermolecular distance, which can be significant for continuum simulations of fluids in nanoscale pores.
The study was implemented in the framework of the Basic Research Program at the National Research University Higher School of Economics (HSE University) in 2021.

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Predicting hydrocarbons properties at pressures up to 1 GPa using molecular dynamics methods

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The ability to predict the hydrocarbon liquids properties is of great industrial interest, since they are components of oils and fuels. In this work, we apply classical molecular dynamics methods to calculate the equation of state and self-diffusion and viscosity coefficients of the linear and branched alkanes and aromatic compounds [1–4]. The interatomic force fields are compared by their ability to predict the experimental data. The molecular dynamics methods are used to predict the shear viscosities of hydrocarbons in the pressure range from 0.1 MPa to 1 GPa. Blindly predicted viscosity values for isononane match the experimental data measured later. We demonstrate the universal scaling between the viscosity and diffusivity at pressures up to 500 MPa.

The work is funded by the Russian Science Foundation (grant No. 17-79-20391).

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Surface tension of interphase borders of alkanes

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The method of molecular modelling is used to calculate the value of surface tension of borders between liquid and gas phases of methane-ethane mixture.

Collective motion of atoms in solids

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The work is devoted to the study of the collective motion of particles in solids and liquids of Lennards-Jones systems using the method of molecular dynamics. We continue started in [1] analysis of pair correlator

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

which characterizes correlation of particle motion. Here $\mathbf{r}_i(t)$, $\mathbf{r}_k(t)$ are the radius-vectors of particles i and k located at a distance $R\pm\delta$ at the initial time t. Brackets $\langle\ldots\rangle_R$ means averaging over all selected pairs of particles.

We found that the correlations in crystals is much greater than in liquids. The temperature dependence $\mathrm{CC}(T)$ demonstrates the hysteretic behavior varying along the isochore. Correlator values are higher in crystal with defects than in pure one. In addition, its values increase during phase transitions and crystal lattice reorganizations. Radial dependence $\mathrm{CC}(R)$ exhibits crystal structure in more sensitive way than radial distribution function.

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Collective dynamics in supercooled glass-forming aluminium-based melts

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The point of phase transition in a substance, despite its exceptional influence on the behavior of a substance, is not special for its thermodynamic functions [1]. Any phase can exist, at least as metastable, and on the other side of the transition point; thermodynamic inequalities at this point are not violated within the relaxation time. Preliminary analysis of metastable fluids [2] revealed features in the region of phase transitions for two-particle motion correlators [2,3], describing the collective dynamics of particles in various models of particle interactions.

In this particular work, the temporal behavior of motion correlators observed in deep supercooled state of aluminium-based melts near glass-transition temperature [4,5]. The analysis shows a change of dynamical structure till the relaxation processes of vitrification and gives vitrification temperature which consistent with volumetric and other analysis methods [6].

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The polarization impact on oxygen diffusion in zirconia

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Zirconium dioxide is used in many technological areas. Particularly, it is a catalyst for chemical reactions, thermal barrier coating material and the electrolysis process component. For high-temperature electrolysis, its resistance to high temperatures and high diffusion coefficient are essential. We study the influence of ion polarization on the diffusion coefficient at high temperatures. Buckingham–Coulomb potential simulated particles interaction, the polarization mechanism is reproduced by the Core-shell model [1]. Each ion is divided into two particles: a core and a shell, interacting with each other according to the equation of a harmonic oscillator. The diffusion coefficient is calculated using the Einstein–Smoluchowski formula, the temperature dependence is fitted using the Arrhenius relation. It is found that the temperature dependence of the diffusion coefficient for a system with polarization extrapolates the experimental data well [2]. The system without polarization is significantly further from experimental data. Also, in the system without polarization, melting is not observed at temperatures exceeding the real melting point.

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Molecular dynamics study of uranium-dioxide sintering process

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Uranium dioxide has received a lot of attention due to its unique nuclear properties and its various applications in nuclear industry Nowadays, there are many works devoted to sintering of uranium dioxide. However, the influence of crystalline misalignment between two nanoparticles on the process has not been sufficiently studied. In this work we study the process of sintering of UO_2, in particular, the influence of the grain boundary on the rate of this process, using the molecular dynamics method. Computations are performed on 2–4 cylindrical nanoparticles in the conditions of NVE ensemble, with the interatomic potential [1]. Periodic boundary conditions are used to avoid surface effects. Coefficients of grain-boundary and surface diffusion were obtained for four different misaligned angles. From the temperature dependence of the diffusion coefficients, the activation energy for each mechanism was calculated. Three theoretical models were used to obtain the total relative diffusion coefficient. The consistency of two-particle and many particles models has been investigated through the comparison of shrinkage and densification data, calculated using the first and the second model respectively. All computations were performed using LAMMPS package [2].

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Molecular dynamics study of the glass transition temperature and elastic properties of the Zr–Nb amorphous alloy

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For Zr–Nb alloy, the crystalline phase has been well studied. For the amorphous phase, a detailed study of the structure and structural criteria of glass transition [1] was previously carried out, but the non-structural criteria and elastic properties remained unstudied. The study was carried out using the molecular dynamics (MD) method with ADP-potential [2]. The calculations were carried out for Nb percentages ranging from 25 to 75 percent and a cooling rate of 11 K/ps. The glass transition temperature for different percentages of Nb was determined by varying the dependences of viscosity, heat capacity and diffusion coefficients on temperature. The data obtained are in good agreement with each other. The elastic properties of amorphous Zr–Nb were also investigated. Young's modulus for different percentages of Nb was determined. It is shown that the modulus of elasticity increases with decreasing free space in the structure, which is consistent with the assumed deformation mechanism of amorphous alloys. The presence of pressure hysteresis under compression and reverse tension, as well as its dependence on the percentage of Nb content is also consistent with the assumed deformation mechanism of amorphous alloys.

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Study of the threshold crystallization rate of Si–Al and Si–Au nanoparticles with molecular dynamics method

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In connection with the development of the laser printing methods, it is important to study the structure of silicon nanoparticles with impurities of gold and aluminum, since such objects demonstrate various practically important optical and electromagnetic properties depending on the structure obtained upon cooling [1]. In this work, a study of the crystallization of three-dimensional particles was carried out. The method consists in cooling the melt to room temperature. Next, the structure of the nanoparticles was analyzed and the threshold cooling rate required for crystallization was calculated [2]. A wide range of metal impurity concentrations was considered. There are presented the values of the threshold velocities for nanoparticles with a radius of 20 nm. The data obtained are consistent with the images obtained during the experiment for Si–Au nanoparticles. The results of the work are aimed at predicting the physical properties of nanoobjects of a similar structure. All calculations were carried out using a new potential (developed for the LAMMPS package [3]), which was created in the last year, which correctly describes such systems [4].

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Point defects and self-diffusion in temperature-stabilized bcc metals

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Point defects are responsible for self-diffusion processes in crystalline solids. According to the classical concepts, diffusion in normal metals mainly occurs due to the formation and migration of monovacancies. The diffusion coefficient D can be expressed by the Arrhenius equation, where the activation energy is correlated with the melting temperature. However, the characteristic values of correlation coefficient in some anomalous bcc metals (Ti, Zr, Hf, U, Ce, Gd, La, Pr, Pu, Yb) are 1.5–2 times smaller than in normal metals. The pre-exponential factors are several orders of magnitude too small. The strong non-Arrhenius dependence of the diffusion coefficient is additionally observed for bcc Ti and Zr, as the temperature range for their phase stability is quite large. One common feature for all anomalous metals is that the bcc phase exists only at high temperatures or pressures and is mechanically unstable at 0 K.
In this work, I obtain the temperature dependence of the self-diffusion coefficient in bcc titanium directly from molecular dynamics (MD) calculation. MD simulations indicate that both vacancies and self-interstitials contribute to diffusivity in bcc Ti. The resultant self-diffusion coefficient is non-Arrhenius, but shows less curvature than observed in most experiments [1]. I also show that the formation free energy of self-interstitials in bcc uranium is much smaller than for vacancies. [2].

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Verification of mathematical model of solid with defects under dynamic loading

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The previously developed mathematical model of a solid with mesoscopic defects was validated on the comparison with experimental data from dynamic tests, including the Hopkinson–Kolsky test and shock-wave loading. The proposed constitutive relations (equations of state) allow the description of the deformation behavior of typical elastoviscoplastic materials (metals and alloys) in a wide range of strain rates, temperatures and stresses. Techniques for estimation of identifying parameters of the model have been developed and based on solving a number of independent problems of minimizing the residuals between the calculated and experimental data. During identification procedure, both literature data and author's experiments were used. An experiment was carried out on high-speed collision of a cylindrical sample with a rod (Taylor–Hopkinson test) combined with registration of the temperature field. The comparison was carried out by numerical modeling using the finite element method in both three-dimensional and axisymmetric formulations. The results of numerical calculations are in good agreement with the experiments performed: the shape of the rod after collision and the measured temperature (dissipation of mechanical energy during inelastic deformation) coincide. This testifies to the adequacy of the developed mathematical model and indicates the possibility of its application for solving problems in solid mechanics.

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Charged ions in magnetic field: Effects of the stochastic forces

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Ions are the most important components in biological systems other than deoxyribonucleic acid and proteins. They have an important role in signalling processes, are functional parts of the proteins, etc. Thus it is crucial to understand their behavior in various conditions. In this work, we consider a charged ion in a uniform magnetic field and confined potential. Also, it is coupled to a thermal bath, which will resemble the biological environment. To get non-trivial results we add colored (correlated) noise and add memory to the friction forces.

We write down the generalized Langevin equation (GLE) for the ion. The colored noise complicates things, and we derived approximate analytical results only for a limited set of potentials. However with the help of numerical methods we tested the validity of these results for more complicated nonlinear potentials.

It turns out that for a certain range of parameters of the model, the dynamics of the particle is deterministic despite high friction and stochastic forces from the environment. We tested this result by solving GLE numerically. These equations are stochastic differential equations, therefore advanced numerical methods were used.

THERMOS Toolkit: Self-consistent solution of the radiation transfer equation with kinetics in one-dimensional geometries

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A software module has been developed to calculate the properties of an one-dimensional non-local thermodynamic equilibrium (non-LTE) plasma. Numerical simulation is produced within a consistent solution of the radiation transfer equation with a system of rate equations in the collisional-radiative equilibrium approximation. Modeling can be performed in three simplest one-dimensional geometries (an inhomogeneous infinite flat layer, a ball and an infinite cylinder inhomogeneous along the radius). The development of the module and its inclusion in the THERMOS Toolkit [3] has made it possible to significantly expand the range of problems to be solved for modeling the properties of plasma under the non-LTE conditions.
The reported study was funded by the Russian Foundation for Basic Research (project No. 20-01-00485). Calculations have been performed at high performance computers K-100 (Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences) and MVS-10P (Joint Supercomputer Center of the Russian Academy of Sciences).

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

THERMOS Toolkit: Taking into account non-equilibrium plasma effects in radiative hydrodynamics calculations

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Modeling of non-local thermodynamic equilibrium (non-LTE) plasma is a complicated problem and although modern methods of atomic physics are capable of providing quite accurate results, the in-line use of precise models in radiative hydrodynamics simulations is still a rare phenomenon. Most of the practical plasma dynamics simulations are still run at the expense of accurate atomic physics simulations in favor for hydrodynamics and its associates. A commonly spread approach is to use one the most suitable for the task at hand approximation for opacity and equation of state calculations. Our research group has proposed more advanced method [1], that utilizes a certain pair of tables for two limiting cases. This model effectively takes into account the spatial finiteness of laboratory plasma, however the spectral features of local radiation field are amiss. In this report we investigate different radiation field limiting cases and interpolation parameter variations and outline the area of applicability of this method. The reported study was funded by the Russian Foundation for Basic Research (project No. 20-01-00485). Calculations have been performed at high performance computers K-100, K-60 (Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences) and MVS-10P (Joint Supercomputer Center of the Russian Academy of Sciences).

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Numerical investigation of the dense photoionized aluminum plasma

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On the Linac Coherent Light Source (LCLS) x-ray laser facility the solid-density aluminum was irradiated with ultrashort high-intensity monochromatic beams of x-ray photons [1,2]. The measured spectra contain lines corresponding to K-shell emission which is explained by the Auger effect and the photoionization of electrons from the inner shell.

For the numerical simulation of this experiment, a physical model is required that will include both the nonstationary kinetics of the populations of ion species and the density effects. The corresponding model was implemented in the THERMOS Toolkit [3], which made it possible to reproduce the measured spectra with good accuracy.

The reported study was funded by the Russian Foundation for Basic Research, project No. 20-01-00485. Calculations have been performed at high performance computers K-100, K-60 (Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences) and MVS-10P (Joint Supercomputer Center of the Russian Academy of Sciences).

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Wave packet molecular dynamics density functional theory simulations of shock-compressed deuterium

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A new wave packet molecular dynamics (WPMD) density functional theory (DFT) simulation method is applied to study the shock-compressed deuterium. The method is based on the WPMD and DFT. It allows to study nonideal plasmas and warm dense matter accounting for simultaneous dynamics of electrons and ions, electron–ion relaxation, plasma conductivity and interaction of plasma with the laser irradiation. In this report, we condenser mainly thermodynamic properties of the shock-compressed deuterium to validate the WPMD-DFT method. In this approach, the electrons are represented as Gaussian wave packets whereas the Hartree approximation for the many-body wave function is used. The exchange and correlation effects are treated using an additional energy term taken from DFT. This term is determined by an exchange-correlation functional and a correction to the kinetic energy. It is calculated via integration over the mesh values of the function that depends on the electron density. The local electron density distribution is determined by the positions and widths of the wave packets. The proposed approach is meant as a replacement for the antisymmetrized WPMD (AWPMD) method which is more time consuming. The WPMD-DFT method is applied for direct simulation of deuterium shock compression. The simulation is performed as a series of compression and relaxation stages. The convergence of simulation results as a function of compression speed is studied. In addition, the WPMD-DFT method is used for isentrope calculation via Zel'dovich's approach. The results are compared with experimental data and other quantum molecular dynamics simulations.

Atomic volumes of elements: Modern computational methods and experiment

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It is well known that atomic volumes of elements at normal pressure exhibit oscillatory behavior with the rise of atomic number [1, 2]. It was also predicted [2] that the curve of atomic volumes should become monotonic at very high pressures (100 Mbar) due to the disappearance of electron shells. At such pressures semiclassical models are valid; in particular, the Thomas–Fermi model [3] states that all atomic and thermodynamic properties can be described by self-similar relations. It was also shown [4] that molecules are unstable in the Thomas–Fermi approximation so that chemistry is impossible at high enough pressures. In the present work, we apply modern theories to the calculation of atomic volumes at normal and higher pressures. We use pseudopotentials, full-potential density functional theory and average atom models to construct the dependencies of atomic volumes on the atomic number at 1, 10 and 100 Mbar. We compare our calculations with shock-wave experimental data as well as with much more accurate diamond anvil cell measurements. The work is supported by the Russian Science Foundation (grant No. 20-42-04421).

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Many-body quantum dynamics by means of the time-dependent density functional based reduced density matrix theory

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We evaluate the density matrix of an arbitrary quantum mechanical system in terms of the quantities pertinent to the solution of the time-dependent density functional theory (TDDFT) problem. Our theory utilizes the adiabatic connection perturbation method of Görling and Levy [1, 2], from which the expansion of the many-body density matrix in powers of the coupling constant λ naturally arises. We then find the reduced density matrix $\rho_\lambda(\mathbf{r}, \mathbf{r}', t)$, which, by construction, has the λ-independent diagonal elements $\rho_\lambda(\mathbf{r}, \mathbf{r}, t) = n(\mathbf{r}, t)$, $n(\mathbf{r}, t)$ being the particle density. The off-diagonal elements of $\rho_\lambda(\mathbf{r}, \mathbf{r}', t)$ contribute importantly to the processes unaccessible via the density, directly or by the use of the known TDDFT functionals. Of those, we consider the momentum-resolved photoemission, doing this to the first order in λ, i.e., on the level of the exact exchange theory. In illustrative calculations of photoemission from the quasi-two-dimensional electron gas and isolated atoms, we find quantitatively strong and conceptually far-reaching differences with the independent-particle Fermi's golden rule formula [3].

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Territorial protection utilising seismic barriers using granular metamaterials

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The paper presents an idea behind the utilisation of seismic barriers for territorial protection. The practical actuality of the approach is vividly demonstrated–no other contemporary seismic protection system can deliver the necessary protective properties combined with economic efficiency and a possibility to retrofit protection to shield the existing structure. Presented simulation results show that utilising seismic barriers filled with heterogeneous granular hyperelastic material for the rather extent area, magnitudes of displacements and accelerations, arising as a result of a seismic event, can be easily reduced by a factor of 4–6. It is shown, that the unique properties of granular metamaterials provide a very efficient dissipation of wave energy inside barrier in addition to reflection of energy and transformation of potentially dangerous surface wave energy into much less harmful energy of bulk waves.

Numerical models of non-stationary concrete behavior

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Mechanical and mathematical models of concrete deformation and destruction was reviewed. A list of concrete models suitable for numerical modeling of non-stationary concrete behavior at the modern level of computer development was determined [1], taking into account the presence of constants of models and their adequacy in describing the behavior of concretes under low-speed impact.

A new variant of the defining equations is proposed. These equations are a development of widely used concrete models: the deformation theory of plasticity by G A Gineev and the Holmquist–Johnson–Cook model. For these models, the most used and experimentally justified sets of constants are presented. Several correlation relationships allowing to estimate constants of models for developed high-strength concretes in case of absence of corresponding experimental data are given.

Numerical algorithms for realizing the governing equations of concrete models have been developed, tested and described in detail. Numerical models were validated by comparison with experimental data on penetration depth and ballistic curves for the axisymmetric case. Satisfactory agreement was obtained on the results of the calculations with the experimental data.

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Numerical solution of inverse problem to determine parameters of non-stationary load from measured parameters of shell reaction

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The implementation of up-to-day technical requirements for missile and space technics is impossible without ensuring the protection of their constructions from the mechanical action of radiation and the impact of compact solids. Both types of actions cause non-stationary deformations of constructions and their subsequent destruction. In the case when the construction is protected by a multilayer porous package, the wave stage of deformation is generally not dangerous and destruction occurs at the shell stage. At the same time, the features of the mechanical action of radiation and the impact of bodies are leveled, and as a result, everything is reduced to the effect of one-sided non-stationary pressure.on the surface of the protected construction.

This work is devoted to the determination of pressure parameters (its impulse and duration) from the measured reaction parameters of the thin-walled construction (non-stationary deflections and deformation fields). The solution of this inverse problem was made numerically using regularization methods and the results of multivariable calculations of non-stationary deformations and deflections of multilayer panels and cylindrical shells according to the method [1].

This work was supported by the Russian Foundation for Basic Research (No. 19-08-00606).

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Simulation of the polymeric materials high speed impact

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Polymer materials, in particular, polymethyl methacrylate (PMMA) are widely used as structural elements in the study of shock wave and detonation processes in various materials. In this regard, mathematical modeling of the behavior of polymer materials under conditions of high strain rates is relevant. Various empirical models are used to describe plastic flows. In this work, a mathematical model of an elastoplastic medium is built on the basis of the Prandtl–Reis model of plasticity [1, 2], a distinctive feature of which is the absence of empirical constants. Namely: in the Prandl–Reis model, the equations for the stress deviator tensor components have the same form as the equations for stresses in the Maxwell model of a viscoelastic medium [3], however, unlike the Maxwell model, the Prandtl–Reis model does not require the introduction of an additional fitting parameter—viscosity. Also, a low-parameter equation of state in the Mie–Grüneisen form is constructed, which adequately describes the behavior of a polymer material under dynamic loads. For the numerical solution of the proposed mathematical model, a semi-analytical method was used [3]. The verification of the mathematical model was carried out on the basis of experimental data [5], which showed that the constructed mathematical model gives a correct description of shock-wave processes in polymer materials.

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Software package for calculating two-dimensional flows in Lagrangian coordinates

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Researches in the field of continuum mechanics are based on the use of various software packages now. Commercial programs allow solving a wide range of applied problems, but the existing physical and mathematical models are constantly being supplemented and complicated, which makes it impossible to quickly improve the modeling tools. On the other hand, the development of our own software systems mostly solves the above-described disadvantages. The creation of a software product that allows solving computational fluid dynamics problems with an architecture that allows you to quickly modify the source code for solving specific problems is an urgent task. In this work, an algorithm for calculating two-dimensional flows in Lagrangian coordinates is numerically implemented, based on the Kuropatenko method [1,2], the use of which to determine auxiliary quantities on the faces of grid cells allows, on the one hand, to correctly describe the energy dissipation at the shock front, and with on the other hand, to preserve entropy on smooth flows. Reconstruction of the Lagrangian grid is based on the method [3], and consists in recalculating all parameters from the old grid to the new one in accordance with the laws of conservation of mass, momentum and energy. The developed software package has shown its efficiency when testing on problems with an analytical solution.

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Regression analysis on artificial roughness shape impact on heat transfer enhancement in a circular pipe

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Results of numerical modeling and regression analysis are presented for turbulent airflow inside a circular pipe provided with artificial roughness of squared and delta-shaped elements. The effect of the parameters under consideration (roughness height and pitch, flow Reynolds number) on heat transfer enhancement, pressure drop, and total performance is assessed. A regression problem of predicting these values given input parameters is solved with deep learning algorithms. The first part (126 samples) of the acquired dataset of numerical results for squared elements is utilized for training a 3-layer feedforward neural network. Predictions of this model are then merged with 20 other samples (the results for delta-shaped elements), and proceeded to 1-layer network, representing model stacking technique [1] widely used in terms of the lack of data. Both models are showing promising results (less than 2% mean percentage error on k-fold and hold-out validation) for industrial applications.

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Analytical and numerical modeling of non-stationary flow of the bottom part of the ascending swirling gas flows

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There is a number of largely destructive natural phenomena such as tornadoes and tropical cyclones. The bottom part of the ascending swirling flow is constructed analytically and numerically. For the gas dynamics system of equations allowing for gravity and Coriolis force the Cauchy characteristic problem with initial conditions on the $z = 0$ horizontal plane is considered. Herewith the value of the vertical component of the gas velocity vector is $w = 0$, that is gas does not flow through the $z = 0$ plane. In the case of general spatial isentropic currents, the $z = 0$ impermeable plane is the contact characteristic of multiplicity of 2. For the considered problem with the initial data at $z = 0$ to have a single solution, one should establish the two auxiliary conditions on the other surface. Let us consider the radial component of the gas velocity vector $u = -\text{const}$ on a non-zero radius cylinder, and the circumferential component is $v = 0$. The decision of the problem is constructed in the form of the interval in powers of z. For a numerical solution, a modified characteristic method is used where the grid is set before the start of the counting.

Partial solution of a linearized system of equations of gas dynamics taking into account the action of the Coriolis force

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Due to the non-linearity of the system of gas dynamics equations, the construction of its solutions is quite time-consuming. This was the reason for the linearization of the system of gas dynamics equations on its exact solutions [1]. In this paper, if we do not take into account the action of gravity, we present a linear system of partial differential equations based on an exact solution. The influence of gravity is not taken into account when studying gas-dynamic flows in the bottom parts of natural ascending swirling flows, in which the gas parameters do not strongly depend on the height. A concrete solution for a linearized system in the form of a traveling wave propagating in different directions is constructed. The presence of several traveling wave propagation velocities for a system of gas dynamics equations is a rather unexpected fact. This happens only in the case of multicomponent media [2]. Obviously, this fact is due to the fact that the system of equations of gas dynamics takes into account the action of the Coriolis force. The obtained solution is modeled by the Runge–Kutta numerical method of the fourth order of accuracy.

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Direct cascade numerical simulation in two-dimensional turbulence accompanied by energy flux

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In this paper, we numerically study two-dimensional turbulence in a bounded region of given dimensions in an inviscid medium under the action of an external force. The characteristics of the turbulent flow, such as the evolution of kinetic energy and enstrophy, are given. Spectral characteristics of the flow are shown, revealing the process of energy transfer at different scales of the problem. The numerical experiment was carried out using the HYPERBOLIC_SOLVER software package developed by the authors. This package implements a generic approach to the construction of computer programs. To solve the problem, the hydrodynamic part of the package is used, which implements the numerical scheme of the simplest linearization of the Godunov method. This scheme has a second order of accuracy in space. In general, the problem under consideration belongs to the class of problems whose solution is necessary for understanding the mechanisms of the emergence and development of a two-dimensional turbulent flow and its internal structure.

Features of the self-oscillating mode of fluid filtration in porous media

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Filtration processes for two-phase fluids (mixtures of hydrocarbons, steam–water mixture) in porous media can be unsteady. Of particular interest are the so-called self-oscillating filtration modes in which stable fluctuations of the fluid flow rate are observed under constant boundary conditions. Such modes are recorded both in the course of bench experiments [1] and in mathematical modeling of unsteady two-phase filtration [2]. The emergence of such filtration can have a complex mechanism associated, among other things, with the lack of thermodynamic equilibrium in the zones of phase transformations [3]. The assumption of local thermodynamic equilibrium is characteristic of many mathematical models used to simulate the processes of unsteady filtration in porous media. However, the applicability of this assumption is questionable. It is possible to solve this problem by developing a mathematical model that takes into account the nonequilibrium processes. The development of methods for modeling non-stationary filtration can be of practical importance, since in the long term it would allow more efficient exploitation of gas condensate fields and sources of geothermal energy.

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Numerical method for modeling the flows of reacting media

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High-intensity flows are characterized by the appearance of features such as shock waves—regions comparable to the molecular mean free path, in which the gradients of gas-dynamic quantities tend to infinity. For a correct description of such processes, the numerical method must include the mechanism of entropy growth at the shock front. As such a mechanism, the proposed method uses a modification of the well-proven method of V F Kuropatenko [1] for calculating strong shock waves. This modification allows using the Kuropatenko method in Eulerian coordinates.

At the moment, there are no published works presenting the modeling of flows of chemically reacting media using the Kuropatenko method. In this work, the approach presented by Pigasov was used to simulate chemical transformations. The used sets of chemical reactions and their parameters are described in the kinetic mechanisms of Matveev [2] and Babushok [3].

This paper presents a mathematical method and a model of a multicomponent continuous medium for high-intensity flows of reacting media simulation. The results of modeling the ignition and detonation of a hydrogen-air mixture in a shock tube showed good agreement with experiment [4].

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Nucleation of soot nanoparticles from polycyclic aromatic hydrocarbon precursors

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Understanding of the soot formation process is crucial for reduction of harmful emissions from combustion and also for synthesis of various important carbon structures. It is widely accepted that nucleation of carbon nanoparticles in flames comes via intermediate stage of formation of polycyclic aromatic hydrocarbons (PAHs) and their dimerization, but still precise physical and structural properties of the nanoparticles in the early stages of formation and nucleation mechanism still remain unknown. In this work we describe nucleation kinetics of soot particles formed from large PAH structures with more than 60 atoms. Molecular dynamics simulations with reactive potential ReaxFF [1] were performed in temperature range 2000–2700 K. Structure of soot nanoparticles is examined by comparing parameters such as hybridization, [H]/[C] ratio, distribution of carbon fringe length and tortuosity. In addition, we examine how formation temperature affects the particle morphology and thermal stability.

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Kinetics of carbon soot growth from polycyclic aromatic hydrocarbon precursors: Atomistic modeling

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Soot formation have a great impact on such processes as fuel combustion and synthesis of carbon structures. Nevertheless, the formation and growth of soot structures have not been understanded well [1, 2]. The collisions between soot particles and different hydrocarbon molecules are valuable for understanding the process of soot particles growth. We examine how the morphology of soot nanoparticles formed at different temperatures (in the range $T = 2250$ to 3000 K) influence their ability to adsorb PAHs (polycyclic aromatic hydrocarbons) from the gas phase and how it affects the growth kinetics in general. This way, we study the energy of the interaction between PAH molecules and soot. The results were obtained using LAMMPS with ReaxFF [3] potential.

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Disentanglement process during deformation of carbon nanotube-filled polyethylene

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Properties of polymer nanocomposites differ from properties of pure polymer. Addition of the nanoinclusions to the polymer melt affects the mobility of polymer molecules and creates additional topological limitations. The mechanical properties of the model system of a polyethylene matrix with carbon nanotubes were investigated within the method of molecular dynamics. The method of calculating the primitive path [1] was used to analyze the change in the topology of the entanglements of the polymer chains during uniaxial deformation for both systems–the pure polyethylene and the nanocomposite. It has been demonstrated that the presence of the carbon nanotubes (CNTs) made polymer matrix more disentangled. Moreover, the variation of the CNTs length affects the number and the lifetime of the entanglements. Analyzing the data, an attempt is made to find the connection between the changes in elastic properties and the pore formation [2] arising from the addition of nanoparticles dynamics and the process of disentangling interchain kinks.

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Structural properties of liquid carbon: Atomistic modeling

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Experimental data on the melting curve of graphite and thermodynamic properties of liquid carbon remain controversial despite the long history of investigation [1]. The results of several dozen experimental works cover the wide span from 3800 to 5000 K for the graphite melting temperature that is essentially larger uncertainty than the errors of individual experiments. Liquid carbon remains the source of several unsolved questions related to its structure, pressure–temperature regions of stability, and the possibility of the existence of liquid–liquid phase transitions. Extending our previous results on the melting kinetics and parameters of graphite melting line [2], we study properties of liquid carbon on the basis of molecular dynamics with machine learning-based Gaussian approximation potential (GAP) for carbon [3] and density functional theory (DFT). The properties (such as density and atom hybridization proportions) modeled with GAP-20 are in excellent agreement with DFT data. The structural properties and atom hybridization for liquid carbon at $T = 5000$–6000 K and $P = 1$–3 GPa are calculated. We demonstrate that in the given range of temperature and pressure the majority of atoms are sp-hybridized and form one-dimensional chains.

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Graphics processing unit portability of atomistic modeling codes

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LAMMPS [1], GROMACS [2] and OpenMM [3] provide support for CUDA and OpenCL technologies. The new ROCm HIP technology delivers maximum performance on AMD graphics processing units (GPUs). In our recent work [4], a backend for ROCm HIP was added to LAMMPS. In this study, platform-dependent errors in the source code of the LAMMPS package were found and fixed. There was found a huge increase in memory consumption using the Tersoff potential with OpenCL, which severely limits the available size of systems. To solve this, a cross-platform implementation of the radix sorting algorithm for the GPU was created, which allowed us to transfer the calculation of the neighbors lists to the GPU. This reduced the memory consumption of the Tersoff model by 6 times. To provide the ability to compile the OpenCL backend on modern AMD accelerators, corrections were made in this work to improve compliance with the OpenCL 2.0 standard. Porting of the VASP [5] package to the ROCm HIP framework for using AMD hardware is discussed. The main part of the code is written in Fortran, the part related to CUDA is written in C and uses the old versions of cublas and cufft libraries. The talk describes a method of adapting such code for AMD infrastructure.

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Mathematical modeling of rf plasma flow at low pressures in vacuum chamber with charged sample

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Radio friquency plasma at low pressures (p = 13.3–133 Pa) with gas flow is effectively used for modifying the surfaces of materials of organic and inorganic nature [1]. This type of plasma has the following properties: degree of ionization is 10^{-4}–10^{-7}, electron density is 10^{15}–10^{19} m^{-3}, the electron temperature is 1–4 eV, the temperature of the atoms and ions in the bunch (3–4) $\times 10^3$ K in the plasma jet (3.2–10) $\times 10^2$ K. The main feature of rf plasma flow at low pressure is that for neutral component plasma flows in a transitional mode between the continuum mode and free-molecule flow, the charged components can be approximated of continuous medium [2–4]. Calculations of the flow of rf plasma with sample are completed. The distributions of the velocity modulus, pressure and temperature of the carrier gas argon and the electron density, electron temperature, electric field are obtained. The reported study was funded by the Russian Science Foundation, according to research project No. 19-71-10055.

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Molecular dynamics study of the effect of the substrate temperature on the self-assembly of a copper nanofilm in a gas discharge

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Copper-based nanostructures can serve as an alternative to noble metals for their use as catalysts in a number of chemical processes [1]. One of the methods for obtaining metal nanostructures is the impact on a massive sample of high-energy ions of a gas-discharge plasma with subsequent sputtering and deposition of individual atoms and (or) metal clusters on the substrate [2, 3]. This method can be improved with the help of computer simulation, which makes it possible to identify the optimal parameters without field experiments. In this work, using the molecular dynamics method, we simulate the sputtering of a copper target and the subsequent formation of a copper nanofilm on a silicon substrate. The process parameters corresponded to the conditions in a low-pressure gas-discharge plasma. The obtained values of the sputtering coefficient correspond to the experimental data. The studies were carried out for various values of the substrate surface temperature.

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Investigation of low-pressure ion cyclotron range of frequencies discharge in a self-consistent formulation

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A self-consistent model of a low-pressure ion cyclotron range of frequencies discharge in a self-consistent formulation is constructed. The model includes Maxwell's equations rearranged to a system of elliptic equations for the squares of the moduli of the electric E and magnetic H strengths [1, 2], the electron balance equation and the electron energy conservation equation. Transfer coefficients are functions of electron temperature. The electron balance equation is considered as a nonlinear eigenvalue problem with boundary conditions of the third kind. The spectral parameter is the characteristic value of the electron temperature T_e^*, defined as a solution of the nonlinear equation $\lambda_0(T_e^*) = 1$. Here λ_0 is the smallest eigenvalue of the Sturm–Liouville problem for electrons. Based on T_e^* and the system of equations, the values of $E_R = E(R)$, $H_R = H(R)$, $n_{e0} = n_e(0)$, where R is the discharge radius, are found. The dependences of n_e, E, H, T_e^*, H_R on the frequency f, pressure p, and discharge radius R are investigated. The reported study was funded by the Russian Science Foundation, according to research project No. 19-71-10055.

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Variational-statistical calculation of the gaseous medium density field in the vicinity of a spherical crystalline nanoparticle

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Using a two-level statistical method for describing the behavior of inhomogeneous systems, calculations were performed to determine the micro- and macrostructure, as well as the thermodynamic characteristics of a molecular heterogeneous system consisting of a crystalline nanoparticle, which is in equilibrium with a gaseous macroscopic medium. The interaction between molecules are described using the Lennard-Jones potential. The calculations were performed taking into account the radial spatial relaxation of the parameters of the fcc lattice of a defect-free nanoparticle with site occupation numbers equal to unity ($n = 1$). This means that in a crystalline spherical nanoparticle containing 15 coordination spheres, the presence of thermal vacancies was not taken into account. Near the boundary near the nanoparticle, the radial density profile of the gas medium was approximated using the two-parameter function $n(r_p)$ containing the hyperbolic tangent, i.e., $n(r_p) = a - (a - n_0)\tan(\kappa\Delta r_p)$. Here, p is the coordination sphere index number; a and κ are the variation parameters; n_0 is the value of the occupation numbers far from the nanoparticle, which determines the density of the bulk gas homogeneous medium. At the nanoparticle boundary $p = 15$, and its radius is $r_{15} = 4.38\sigma$, σ is the linear parameter of the Lennard-Jones potential. For example, for argon $\sigma = 0.3405$ nm, so the radius of the nanoparticle is $r_{15} = 1.49$ nm. The functional $\Omega\{n_p\} = F\{n_p\} - \mu\Sigma n_p$ was varied for different values of the parameters a and κ at a temperature of $\theta = 0.6$, which corresponds to a phase transition between a nanoparticle and a gaseous medium.

Phytoplankton colony propagation in the frame of piecewise linear model

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The mathematical model of an infiltrative tumor is regulated to the mechanism of phytoplankton propagation in a channel filled with nutrients. This model consists of reaction-diffusion equations for phytoplankton concentration and nutrient concentration, in which biological interactions are approximated by piecewise linear functions. Within the framework of the one-dimensional approximation, a stable autowave solution is obtained, which moves with a certain critical minimum velocity $u_{\min}$. It is shown numerically that in an unperturbed medium, a phytoplankton wave moving at a velocity $u > u_{\min}$ tends to a stable state with a velocity of $u_{\min}$. The properties of the propagating wave of a phytoplankton colony are compared with the solution of the Fisher equation. The main purpose of the work is to study the features of the propagation of the front of the phytoplankton population in the presence of vortex flow. For this purpose, the nature of the distribution of the phytoplankton colony is studied in a chain of two-dimensional vortices described by the Taylor–Green solution. It is shown that there are three different modes of propagation of the population wave, depending on the intensity of the vortex flow field. The present work was supported by the Ministry of Science and Higher Education of the Russian Federation (project No. 075-15-2019-1878) and the Russian Foundation for Basic Research (project No. 19-01-00768).

5. *Physics of Low Temperature Plasma*

Pressure-produced ionization of non-ideal degenerate plasmas and electrical conductivity

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New experimental facilities allow exploring plasmas at high densities and moderate temperatures where degeneracy effects become relevant [1]. Ionization degree and optical conductivity are interesting physical properties of the plasma in this warm dense matter regime. Quantum statistical calculations [2] and density-functional-theory–molecular-dynamics simulations [3] are used to describe these systems. The effect of degeneracy on ionization potential depression [4] and collision frequency [1, 2] is discussed. Problems in calculating the electrical conductivity are indicated. The authors acknowledge financial support by the Deutsche Forschungsgemeinschaft and the Russian Foundation for Basic Research (DFG–RFBR grant No. 19-52-12039) for the project "Warm dense matter explored with shock wave experiments".

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The investigation of opto-polarizing properties of shock-compressed warm dense matter

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Experimental data from study of optics of shock-compressed plasma is an important cornerstone to construct theoretical models for the description of warm dense matter. Analysis of the response of a dense plasma to the action of an electromagnetic wave can be used as a tool for investigating the validity of physical models describing the behavior of matter under extreme conditions, high temperatures and pressures.

Within this work, the new experimental data on oblique incidence of polarized electromagnetic wave, are presented. The optical properties of strongly correlated plasma were studied in the near-infrared and green spectral regions at a plasma mass density $\rho = 0.82$ g/cm^3. The composition and thermodynamic parameters of the plasma were determined using the modified Saha IV code [1, 2], taking into account the measured velocity of the shock wave in the gas, the equations of states of the gas cell material and the gas under study. The spatial parameters of the plasma transition layer are determined based on the numerical solution of the field equations.

The authors acknowledge financial support by the Russian Foundation for Basic Research (grant No. 19-52-12039).

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Study of nonideal ultracold calcium plasma based on autoionization of Rydberg states

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We have developed a sensitive spectroscopic technique for studying a dilute ultracold plasma using a laser induced autoionization of Rydberg atoms. In our experiment the ultracold ^{40}Ca Rydberg atoms and ions are prepared in a magneto-optical trap by several cw lasers [3]. We detected the plasma with ion and electron densities below 2×10^{-3} m by using our technique. The autoionization resonance is observed as a variation of the resonance fluorescence of the ^{40}Ca ions at a wavelength of 397 nm. The probability of autoionization of atoms is very sensitive to an external electric field [1], which makes autoionization states of alkaline earth metals a promising detector of low electric fields [2].

The present work is supported by the Russian Foundation for Basic Research, project No. 19-32-90197.

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Probing Autler–Townes spectra of strongly coupled lithium $2S_{1/2}$ and $2P_{1/2}$ levels by Rydberg excitation

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Strong long-range interaction between Rydberg atoms modifies the properties and behavior of a dense ensemble of Rydberg atoms. Nonlinear optical effects such as Autler–Townes (AT) splitting [1] and electromagnetically induced transparency (EIT) have been studied in strongly interacting cold and hot atomic samples. In [2, 3], the ground level and the first excited level of cesium are coupled by a strong field and are probed via excitation into a Rydberg level. Interaction between Rydberg atoms leads to sufficient broadening of AT spectra.

In the present work, the effects of the strong long-range interaction of Rydberg atoms on the AT splitting spectrum are investigated. Lithium D1 line transitions are strongly coupled and they are probed by excitation into $70S$ Rydberg states. Interactions between Rydberg atoms excited by the probe beam lead to broadening of the AT spectra. At high concentrations of Rydberg atoms, significant suppression of the excitation of the AT peak at red detuning is observed.

The work is supported by the Russian Science Foundation (grant No. 19-72-00099).

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Singularities of frequency dispersion of permittivity in a disordered Coulomb system with the single-particle Bose–Einstein condensate

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The frequency dispersion of the permittivity of disordered Coulomb systems in the presence of the single-particle Bose–Einstein condensate for nuclei is considered using the linear response theory and the concept of off-diagonal long-range order. It is shown that the superconductivity of nuclei exists in such a system and is manifested in the Meissner effect for a weakly nonuniform low–frequency electromagnetic field. This result offers an opportunity to solve the problem of the presence of the single-particle Bose–Einstein condensate in superfluid He-II based on direct experiments. The Kramers–Kronig relations for the dielectric permittivity of a disordered Coulomb system in the presence of a single-particle Bose–Einstein condensate for nuclei are also obtained [1, 2].

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The thermophysical properties of low-temperature gallium plasma

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Thermophysical properties of a substance (the pressure, the internal energy etc and the electronic transport coefficients) are investigated for more than a century due to their importance for various fundamental tasks and applications. It concerns as well the low-temperature plasma (LTP) region of some elements at the temperatures $T = 10$–100 kK. Appropriate data (calculations and measurements) have appeared in the recent years for a number of practically important elements [1]. However, for Ga (gallium) in LTP state the measurements and calculations of thermophysycal properties have been still absent. There are only *ab initio* simulations along pricipal Hugoniot [2] at relatively high densities $\rho \geqslant \rho_n$ and $T \leqslant 10$ kK, where $\rho_n = 5.905$ g/cm^3 is the density at ambient conditions. At higher temperatures and low densities there are no appropriate data. Thus, it is necessary to fill this gap.

To do it, we have used previously developed model for the considered properties in this area, which has been successfully used for different elements (see [3,4] and references therein). This model was modified to apply it to the low-temperature partially ionized plasma of Ga. So we have calculated the properties under study for Ga LTP (see details in [5]). As far as there are no other data to compare, we have checked only the asymptotic behavior of our results and found that it corresponds to existing theories.

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Estimation of the average ions charge and plasma momentum for vacuum arc plasma

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The parameters of the cathode spot plasma produced by explosive electron emission pulses have been estimated from the critical state properties for various materials [1].

The kinetic energy of the cathode plasma flare has been estimated as $100T_{\rm cr}$, where $T_{\rm cr}$ is the critical temperature of the cathode material. Based on a Saha-like equation and a two-temperature simulation of the explosion of a liquid-metal micro jet, an estimation formula for the average ion charge has been derived, $Z_{\rm av} = 1 + T_{\rm cr}/1$ eV, which fits the available experimental data. This has made it possible to explain the linear relationship between average charge and kinetic energy obtained experimentally for the cathode plasma ions. Using this formula, the previously derived expression for the plasma momentum per transferred charge μ has been simplified to become $\mu \sim 5(M_i/M_p)^{1/2}$ g cm/(s C), where M_i/M_p is the ion-to-proton mass ratio.

Work was supported in part by the Russian Foundation for Basic Research (grant No. 19-08-01249).

Values of critical temperature used herein have been obtained by Academician Professor Vladimir E Fortov, who has suddenly passed away at the end of 2020 and left a scientific legacy in extreme state of matter and plasma physics.

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Hall effect in weakly doped semiconductors

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The Hall effect determines one of the main methods for determining the kinetic properties of various conducting media. To estimate the measured Hall field $E^x_{\rm H}$, it is enough to equate its value to the value of the Lorentz force $F_{\rm Lor}$, acting on free carriers in the volume of the conductor. This "force" interpretation of the phenomenon is usually used, but this definition is approximate. In fact, the stationary Hall state occurs when the accumulation layers $\pm$ appear at the edges $x = \pm d$ of the conducting channel under the action of the Lorentz force $F^x_{\rm Lor}$. This stationary picture is determined not by the "force" requirement $E^x_{\rm H} = F^x_{\rm Lor}$, but by the condition $j_x = 0$ in the direction that limits the channel dimensions, where j_x is the free charge current density in "electrochemical approximation".

Gapped momentum states and shear viscosity limit in strongly coupled mesoscopic systems

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Shear viscosity is the property to resist and diagnose the strength of the interaction between condensed matter constituents. There is a paradox that the low shear viscosity indicates a significant interaction strength [1]. There is estimation of fundamental lower limit $\eta/s = \hbar/(4\pi k_B)$ (universal lower bound). Existence of viscosity limit is related to gapped momentum states (GMS) in open dissipative systems. GMS emerge in liquid viscoelasticity revealing k_g-gaps in dispersion relations with applications in turbulence and non-ideal (dusty) plasma as interplay between propagation, dissipation effects and relaxation time [2]. This corresponds to Fraenkel definition of liquid as condensed matter state retaining structural features of solid and corresponding set of internal (thermodynamic) variables. Structural image of k_g-gap can be introduced as localized shears corresponding to coordinated movement of molecules in elastic field of shear stresses. Statistical thermodynamics of microshear ensemble established criticality type (structural-scaling transition) leading to generation collective modes (solitary and blow-up) as mechanism of k_g-gap related to new spatial and temporal scales. Critical dynamics of microshears collective modes provides anomaly of energy absorption and self-similarity of momentum transfer with power law viscosity asymptotic limits. This asymptotic was supported experimentally at steady state wave fronts in shocked liquids [3].

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Some approach diagnostic electric and kinetic parameters dusty plasma system

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Near the moon surface as a result of interaction with the electrons and ions of the surrounding plasma, as well as under the influence of solar radiation, dust particles acquire an electric charge and become one of the important components of the environment, significantly affecting its properties and dynamics [1]. In the experimental modeling of the near-surface exosphere of the Moon under laboratory conditions, an important condition is the diagnosis of the characteristics of the dusty plasma environment. Of course, the most popular is the visualization of the process, but to understand the changes taking place inside dusty plasma cloud for our experimental chamber we also is used the Langmuir probe and electro-induction grids, tubes or plates. However high voltage when we create dusty plasma and another source of noise have the bad influence during electric measure. Equally important is the use of piezodetectors as low-noise targets for measuring the pulses of the dust component of the lunar dusty plasma environment.

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Manifestations of modulational instability in Earth's dusty ionosphere

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Development of the modulational instability involving dust acoustic perturbations in dusty ionospheric plasma and in dusty plasmas of meteor tails in Earth's ionosphere was considered. The effect of collisions of electrons, ions, and dust grains with neutrals at different altitudes was estimated. It is shown that, in this case, the influence of collisions of electrons and ions with neutrals is usually less significant than the influence of collisions between dust grains and neutrals. It is demonstrated that the effect of the modulational instability on the propagation of electromagnetic waves in the dusty ionospheric plasma is the most significant at altitudes of 100–120 km. The values of the wave vectors of the electromagnetic pump wave at which inelastic collisions with neutrals are important for the development of modulational interaction are calculated. The modulational interaction in the dusty ionosphere is important for the explanation of different phenomena. The absence of observations of low-frequency ionospheric radio noise during such phenomena as noctilucent clouds and polar mesosphere summer echoes caused by the presence of dusty plasmas at altitudes of 80–95 km is explained by suppression of the development of the modulational instability at these altitudes. The role of inelastic collisions with neutrals in meteor tails is also discussed. It is shown, that for typical parameters of dusty plasmas of meteor tails such collisions do not influence on the development of the modulation instability in meteor tails.

Dusty plasmas and Schumann resonances on Earth and Mars

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We discuss possibility of excitation of Schumann oscillations on Mars in comparison with the Schumann oscillations in the atmosphere of the Earth. Dust plays significant role in the radiative and electrical processes in the ionosphere of Mars. Electrification in dust events such as dust devils and dust storms can presumably lead to electric fields large enough for discharges to take place and for existence of oscillations in Schumann cavity. Dust particles present in the atmosphere can influence on the surface temperature, the thunderstorm activity, and the dissipative properties of the ionosphere. In the atmosphere of Mars presence of large amount of dust particles can also influence the surface temperature and dissipative properties of the ionosphere in case when dust particles present at the ionospheric altitudes at high enough densities. As to the correlation between the surface temperature and the fundamental mode of the magnetic field of Schumann oscillations one cannot expect the same on Mars. The main source of energy for Schumann oscillations at the Earth is lightning. In rarified and arid atmosphere of Mars there are no analogues to strong convective meteorological clouds but increases the role of dust events. In Martian atmosphere lightning could probably be excited in dust events such as dust devils and dust storms. The energy released in thunderstorms depends on the frequency and intensity of lighting strokes. The number of dust devils in which the electric field reaches the breakdown value required for the amplitude of the Schumann resonances on Mars to be comparable to the amplitude of the Schumann resonances on Earth is obtained. The amplitude of oscillations in a Schumann cavity on Mars for the cases of dust devils and dust storms as sources of energy is estimated and compared with the parameters of the Schumann resonances on the Earth.

Non-linear screening scaling in a highly asymmetric complex plasma

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We investigate the features of non-linear screening of highly charged macroions by microions in a classical asymmetrically charged complex plasma. Two-component electroneutral systems of finite-sized macroions and oppositely charged point microions in an electroneutral spherically symmetric Wigner–Seitz cell with a central macroion and surrounding microions are studied. This work is devoted to the problem of the relationship between the effective ("visible") charge of the macroion Z^* and its initial charge Z taking into account the effect of nonlinear screening. It is analyzed how this ratio changes with an increase in the charge of the central macroion. The characteristics of two modes are calculated in this dependence of the effective charge on the initial one [1, 2]. The self-similarity of the indicated dependence $Z^*(Z)$ has been demonstrated for various temperatures of the system, macroions concentrations and sizes of macroions [3].

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Confinement impact on the complex plasmas structure

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I will discuss the impact of confining parabolic potential (confinement) on the equilibrium configurations of one- and two-dimensional (1D and 2D) confined strongly coupled complex (dusty) plasmas. In particular, it will be shown that the dust component of the complex plasma is essentially inhomogeneous in such a confining potential: the density of microparticles drops significantly to the system boundaries. This effect qualitatively changes the character of phase transitions (melting and crystallization) in such systems. For example, melting (crystallization) of the confined 2D plasma crystal occurs with the formation of a melting (crystallization) wave, which propagates from the boundaries of the system to its center (in the case of crystallization, it propagates from the center to the boundaries). It has been shown that the equilibrium distribution of the density of the particles is determined only by the softness of the inter particle interaction, which makes it possible to determine the key plasma parameters by non invasive way.

Conversion of energy of fast charged particles into electricity due to non-uniform inert gas ionization

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In [1], it was experimentally found that in e-beam created Ar plasma at atmospheric pressure the current collected by the Faraday cup is directed opposite to the e-beam. In [2, 3], in numerical calculations of a non-self-sustained discharge (NSSD) with an external source of Ar gas ionization, it was shown that the electric field in the anode region changes direction at low voltages applied to the discharge gap. This work is devoted to the experimental and theoretical study of an inhomogeneous plasma created by the e-beam ionization and the determination of short circuit currents and no-load voltages in He, Ne, Ar, Kr, and Xe. The experiments were carried out on the setup [2] with a stationary electron gun with the energy of fast electrons in the range of 50–120 keV as a source of gas ionization. Numerical calculations of the current-voltage characteristics of the NSSD are carried out by the use of the diffusion-drift approach. Both in the experiments and in the numerical calculations, the effect of the electromotive force generation caused by inhomogeneous ionization of an inert gas has been confirmed.

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Kinetics of the production and loss of ion-molecular complexes $H^+(H_2O)_n$ for $n = 1, 2, \ldots, 6$

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The present paper is devoted to studying the kinetics of the production and loss of ion-molecular complexes $H^+(H_2O)_n$ for $n = 1, 2, \ldots, 6$. Atomic positions in such complexes are calculated *ab initio* by the use of global optimization methods. The frequencies of atomic vibrations are calculated, the heat capacities and thermo-chemical parameters of the production and loss reactions of complexes (heat effects and free energies) are determined.

It was found that the vibration frequencies of ion-molecular complexes $H^+(H_2O)_n$ calculated within the harmonic approximation are in poor agreement with the experimental ones; therefore, it is necessary to take into account the anharmonicity of the vibrations. At the same time, the use of the harmonic approximation to analyze the heat effects of reactions and activation energies gives results that coincide with the experimental ones within the measurement errors. It was found that even for small-sized complexes, the heat capacity weakly depends on the arrangement of atoms, and the dependence of the heat capacity of the $H^+(H_2O)_n$ complex on its size is linear even at $n \geqslant 2$. In the calculations, many different configurations of the $H^+(H_2O)_n$ complexes corresponding to different local minima on the potential energy surface were found. It was found that even for small complexes there is a significant number of vibrational modes with low frequencies, close to the frequencies of the rotational motion of water molecules, which suggests a high probability of the participation of vibrational degrees of freedom in the relaxation of collision energy.

Thermodynamic stability of multicomponent nonideal plasma

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In this work, the thermodynamic stability of a multicomponent nonideal plasma is studied. To find pair correlation functions and partial static structure factors, the Ornstein–Zernike integral equations for a multicomponent fluid were used, which were closed with the hypernetted chain approximation. A procedure has been developed for the transition to the one-component approximation for the most nonideal plasma subsystem for the case of any number of plasma components. In this procedure, to determine the pair correlation function in the chosen subsystem, an effective pseudopotential is introduced, which is a function of the remaining direct correlation functions. After a solution for the most nonideal subsystem has been found, the remaining pair correlation functions are determined by the iteration method. Then, the thermodynamic potentials of a multicomponent plasma were determined: internal energy, pressure, free energy, chemical potentials and their derivatives. To find the partial chemical potentials of the plasma components, the method proposed by Hansen [1] was used, which is close to the method of thermodynamic integration. To find the derivatives of chemical potentials, the Kirkwood–Buff approach [2] was used. The data obtained in numerical calculations were used to determine the region of thermodynamic stability of a three-component nonideal dusty plasma.

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A new approach to finding interaction force between charged macroparticles

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The problem of the electrostatic interaction between charged bodies arises from studying dusty plasmas and electrolytes, molecular clusters, and extraterrestrial atmospheres [1]. A possible approach to modelling such systems is to consider a pair of charged dielectric spheres located in a homogenous dielectric medium, which allows to explain the phenomenon of attraction between like-charged macroparticles [2, 3]. However, since the net charge of an isolated ball is equivalent to a point charge located in its center, the series for the interaction force and potential may diverge due to the delta-like contribution to the charge density of the particles. In this work, we avoid such undesirable effect by considering explicit expressions for monopole terms in the electrostatic potential expansion. The approach was developed and tested when calculating the surface charge distribution on a dielectric ball interacting with another charged ball and a point-like charged particle. Results include data for the net interaction force and potential given in comparison with those obtained without separating the divergent terms. This work is supported by the Russian Foundation for Basic Research (project No. 20-32-90054).

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Cleaning dielectric surfaces by the linear electrodynamic Paul trap

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A method against dust pollution of dielectric surfaces is proposed. The dust removal is achieved applying alternating electric fields of special geometry created by the linear electrodynamic Paul traps, which polarize dust particles on the surface of the dielectric and draw them into the interelectrode space of the trap. The captured dust can be contactlessly moved toward the electrodes ends in a special container by an additional constant electric field. The feasibility of the approach was demonstrated by a series of experiments on the contactless removal of aluminum oxide and silica sand sifted through sieves with a mesh size of 400, 280, 200 and 100 μm from a glass surface and solar panels. It was shown that the cleaning method proposed effectively copes with the removal of sand particles smaller than 200 μm in size from a horizontal surface. Through numerical simulation, the capture of a single particle has been analyzed. For a particle of a specific size, the range of product $Q \times U$ necessary for its captureand levitation have been found.

Dynamics of single Janus particle in electrostatic trap

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Active Brownian motion is widespread in nature, in biological and colloidal solutions, in the Earth's atmosphere and plasma with a condensed dispersed phase, as well as in financial models [1]. The movement of the active particle is a superposition of chaotic motion and selfpropulsion. Such particles exhibit a modification of Brownian motion due to the effects of autonomous selfpropulsion (for example, in the case of bacteria) or due to the special nature of their shape or surface, which makes their properties anisotropic. Thus, a very interesting class of artificial swimmers is Janus particles [2, 3]. Experimental data on the active Brownian motion of single Janus particle in electrostatic trap in the radiofrequency discharge plasma under the influence of thermophoretic force, induced by laser radiation, are presented. In this work, we investigated the behavior of a solitary Janus particle at different gas pressures and at different laser powers. The dynamics of active Janus macroparticles and their ensembles has been studied. Trajectories, linear displacements, mean-square displacements and kinetic energies of dust particles were obtained depending on the power of laser radiation. The present research was supported by the Russian Science Foundation (project No. 20-12-00372).

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Nonuniformity of structural and dynamic properties of a dusty plasma monolayer

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Dusty plasma systems have been long considered as a toy model for ordinary condensed matter. Experimentally observed structures of dust particles in a gas discharge plasma are employed to study phase transitions, transport processes and wave phenomena with the methods of video microscopy. At the same time, a set of unique properties makes dusty plasma not just a toy model but an independent object of research [1]. These properties are dissipativity, thermodynamic openness, nonreciprocal character of particle interactions etc [2]. In the present work, we consider a commonly observed case of a dusty plasma system: a monolayer structure in conditions close to typical experimental ones. Behavior of dust particles in the monolayer is studied by solving their motion equations numerically. We show that the action of the horizontal parabolic confinement leads to a nonuniform spatial distribution of structural and dynamic properties of the monolayer [3, 4]. For the first time, we demonstrate that anomalously high kinetic energy of dust particles also has a principally nonuniform spatial distribution in the system and decays with radial distance. Effect of the observed nonuniformity on the scenario of phase transitions is discussed.

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Inhomogeneity of oscillation properties in a dusty plasma monolayer

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In the first approach, experimental dusty plasma structures are described as systems of particles, interacting by the screened Coulomb potential. Their confinement is provided by an electrostatic trap. According to the paper [1] the structural and dynamic properties (e.g., interparticle separation, coupling and Lindemann parameters) of such systems are inherently inhomogeneous. The question of inhomogeneity of oscillation parameters is not studied in detail, so it is of a great interest for researchers. In this work the special case of these systems, called the dusty plasma monolayer, is under consideration. To describe the behavior of particles, their motion equations are solved numerically.
It is demonstrated that oscillation properties of finite systems are fundamentally nonuniform due to their structural inhomogeneity. It is shown that the characteristic frequency of particle oscillations decreases with the increase of its radial distance. We compare the bulk matter and respective homogeneous subsystems of the finite structure in detail to find relations between their oscillation properties. The agreement of results with the theoretical approach [1] and the experiment [2] is reached. Results of the study give relationship between finite structures and bulk matter by oscillation properties. Obtained results are important for the phase transitions research [3].

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Influence of the wake potential on the properties of dusty plasma

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Dusty plasma is a weakly ionized gas that contains condensed matter particles of micron and submicron sizes [1]. These particles usually have a negative charge due to the difference in the mobility of ions and electrons in plasmas. In the absence of external electric fields, ions and electrons are distributed in space radially symmetrically and screen the electric potential of the dust particle. This potential also has radial symmetry and in the linear approximation can be described by the Debye–Huckel expression. However, the overwhelming majority of experiments with dusty plasma are ground-based, and in order for dust particles to levitate, the system is placed in an external electric field. An example of such a system can be a dc or rf discharge with dust particles inside. The presence of an electric field leads to a deviation of the ion distribution in space from the radially symmetric case, and the potential around the dust particle also loses its radial symmetry. The anisotropy of the potential around a dust particle can have a significant effect on the structural and dynamic properties of a system of dust particles. In this work, a theoretical study of the effect of the wake potential on the dynamics of two dust particles in the gas discharge plasma is carried out. It is shown that when the particles are located parallel to the ion flow, the oscillations of the downstream particle are pumped. The influence of the parameters of the complex plasma system on the dynamics of two dust particles is investigated.

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Experimental study of inductively coupled rf plasma in a wide frequency range

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The inductively coupled (ic) rf plasma of the Ar–Hg mixture [1] was studied in a fluorescent tube in the wide frequency range from 1 up to 1000 MHz. A standard frequency for ic rf plasma sources is in the range from 0.05 up to 50 MHz [2]. Plasma was ignited by a capacitive discharge source and then was sustained by an ic rf plasma source. It is observed that plasma glow intensity in the rf coil area depends on rf generator frequency. The dependence had a number of extremes. The effect was observed in airglow discharge, but the rf generator power was not enough to maintain the plasma without a capacitive discharge source. A metal ring was studied instead of a coil. A comparative analysis was carried out between the coil and metal rings. The frequency ranges of plasma supporting for coil and rings were different. These ranges depend on the coil turn lead as well as on the distance between rings. The study was funded by the Russian Science Foundation, project No. 19-71-10055.

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Experimental study of the spectral characteristics of stochastic motion in chain structures of microparticles in a dc gas discharge

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This work presents a new experimental method based on the analysis of the spectral density of random processes, which makes it possible to study nonreciprocal effective forces of interaction between particles in nonequilibrium media. Unlike previous studies, this method does not require special modernization of the experimental setup, external disturbances of the system, preliminary measurements of external fields, or any assumptions regarding the type of interaction. The proposed method was used to recover the derivatives of the forces of interparticle interaction and the external electric field, as well as dissipative forces acting on particles in quasi-one-dimensional dissipative chain systems, by solving the inverse problem of the spectral density of random processes acting in the analyzed system. Approximation of the experimentally measured spectral densities using analytical equations made it possible to determine the derivatives of specific interaction forces and specific external electromagnetic forces. In the entire range of discharge parameters, the effective interaction between particles was nonreciprocal.
This work was supported by the Russian Science Foundation under grant No. 19-12-00354.

Mechanisms of dust particle rotation in stratified dc discharges in inhomogeneous magnetic fields

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We consider the rotation mechanisms in inhomogeneous magnetic fields for dust particles trapped in striations of dc discharges. In general, the mechanisms are the same as for homogeneous magnetic fields. However, in an inhomogeneous axial magnetic field its lines diverge (or converge), and a radial component B_r appears. So we have additional rotation mechanisms. There are two main mechanisms: rotation under action of ion drag and rotation with neutral gas. The ion rotation is due to the ion drift in the crossing electric and magnetic fields, as well as the gradient of ion number density (diamagnetic ion current). In the case of a homogeneous axial magnetic field B_z we have the ion drift in the crossing radial electric (ambipolar) E_r and B_z fields. In an inhomogeneous magnetic field, we get the additional contribution from the crossing longitudinal discharge electric field E_z and radial magnetic field B_r. The gas rotation occurs under the action of eddy currents appearing in striations due to noncollinearity n_e and T_e gradients. Eddy currents in an axial magnetic field cause the gas to rotate. The discharge current in a radial magnetic field can also cause the gas to rotate.

Influence of gas composition on rotation of dusty structures in glow discharge in magnetic field

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Some aspects of the dynamics of rotation of dusty plasma in mixtures of inert gases in a magnetic field are experimentally studied. A method of ion drag force control, based on the fact that the ion drag force increases when a few hundredths of a heavier gas with a lower ionization potential are added to the mixture while maintaining the same discharge conditions. The dependences of the angular velocity of rotation on magnetic field and pressure for discharge conditions under which it is possible to observe stable structures and their rotation in a mixture of helium with a small admixture of xenon are obtained. It is shown that the presence of a small xenon additive significantly enhances the effect of the ion drag on dust particles. In the experiment, new data on the pressure and the proportion in the mixture effect on the angular velocity of rotation of the dusty plasma structure in the magnetic field were obtained.
The work was supported by the Russian Science Foundation, grant No. 18-72-10019.

Comparison of rate of all-round degradation of spherical melamine-formaldehyde dust particles in glow discharge in neon and krypton

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Calibrated melamine-formaldehyde particles are used for studies of dusty plasma, the particles size ranges usually from 1 to 15 μm. In a series of experimental studies carried out with such particles injected in a dc discharge in neon, effects of size degradation and modification of the particle surface have been discovered [1–3]. Now, we present results of an experiment in which changes of particles sizes in a glow discharge in krypton are observed. The dependence of the degradation of the particle size on time is obtained and compared with the one obtained in lighter inert gas (Ne). The comparison performed qualitatively fits the degradation model, which takes into account the process of knocking out the material of particles under the action of bombardment by ions continuously moving to the surface of a dust particle in the process of maintaining its stationary charge. This work is supported by the Russian Science Foundation (grant No. 18-12-00009).

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Observation of a dusty plasma structure in a glow discharge striation in a magnetic field up to 2.2 T

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This report describes a dusty plasma structure formed in striation in a glow discharge when a longitudinal magnetic field is applied. The dependence of the angular velocity of rotation of the dusty structure on the value of the magnetic field in two independent experiments in a range of magnetic field from 0 to 1 T and from 1 to 2.2 T has been obtained. A plot of dependence is presented and combines the two experiments. The mechanisms causing the rotation of the dusty structure in different regions of the magnetic field are described.
Study of the dynamics of rotation of a dusty structure in a magnetic field up to 1 T was carried out with the support from the Russian Science Foundation within grant No. 18-12-00009, the research of the dynamics of rotation of a dusty structure in a magnetic field from 1 up to 2.2 T carried out with the support from the Russian Science Foundation within grant No. 18-72-10019.

Model of plasma of glow discharge in neon at cryogenic temperature

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A model of glow discharge plasma of neon at a cryogenic temperature was developed, taking into account the temperature dependence of the rate constant of chemionization, as well as the formation of molecular ions. The discharge plasma was described in the diffusion-drift approximation. The value of the rate constant of chemionization at a temperature of 77 K was varied with the aim to fit with the experimental data on the pressure dependence of the reduced electric field. The obtained value of the chemiionization rate constant is consistent with the theoretical models available in the literature, however, as far as we know, it has not been previously obtained from the experiment directly or indirectly.
The study was funded by the Russian Foundation for Basic Research (project No. 19-02-00454).

Magnetic and electric resonances in an dielectric rectangular circuit induced by a plane microwave

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Theoretical and experimental investigations of the main electromagnetic resonances excited by linearly polarized microwaves in a rectangular, thin, all-dielectric subwavelength circuit were performed. Displacement and polarization currents induced in this anisotropic circuit are shown to produce resonant magnetic and electric dipoles. The number of resonant modes in a rectangular circuit frame is much greater than in a thin flat ring. The LC magnetic resonances of an all-dielectric rectangular frame are interchanged by the electric ones, forming a complicated spectrum of electromagnetic resonances. These resonances are habitual to the quasi stationary fields in the near zone of the scattering frame. The spectra of these dipoles measured in the near zone of the rectangular circuit frames indicate a variety of resonances subject to the orientation of the frame with respect to the polarization and directivity of the incident radiation. The frames arrangement in three orthogonal planes, normal respectively to the electric component, the magnetic component and the wave vector of the driving wave, illustrate the multitude of narrow polarization-dependent resonances, ensuring the inversion of magnetic inductance and electric displacement in the rectangular frame. These rectangular circuit frames can be used as a multiresonant dielectric metaelements. This research was supported by the Ministry of Science and Higher Education of the Russian Federation (agreement with the JIHT RAS No. 075-15-2020-785).

Resonance scattering of plane electromagnetic waves of GHz range by ring dielectric linear structures

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Resonance backscatter in the fundamental magnetic mode of linear structures consisting of subwavelength dielectric elements in the form of flat thin rings excited by bias currents of an incident plane electromagnetic wave in the gigahertz range is studied. It is shown that the magnetic field at the main resonance frequency for a single ring is concentrated inside the ring and in the near-field zone, whereas for structures consisting of two or more rings the magnetic field is also registered in the far-field zone. The amplitude of the reflected signal at the fundamental magnetic mode increases with an increase in the number of rings. Due to the magnetic coupling of the rings, additional resonance peaks of the scattered radiation occur both in the near- and far-field ring zones. The number of additional peaks increases with an increase in the number of the rings. The main magnetic resonances measured in the spectrum of electromagnetic fields for one and two planar rings coincide with the calculated resonance frequencies. The observed effect of scattering of a plane electromagnetic wave from an ordered system of dielectric rings in the far-field zone at the fundamental resonance frequency of a magnetic dipole makes it possible to use this system to design dielectric mirrors with a negative magnetic response at the fundamental magnetic resonance and at the split frequencies.

Experimental investigations of the microwave electromagnetic waves scattering on the system dielectric ring-plasma

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The resonant scattering on the main magnetic mode of a subwavelength dielectric ring in a system consisting of a glass discharge tube with a low-pressure plasma and a dielectric ring placed on the tube excited by an incident plane electromagnetic wave of the GHz band was studied. It is shown that in the absence of plasma, an intense scattering of the incident electromagnetic wave is observed on the main magnetic mode of the resonant frequency of the ring, which disappears in the presence of plasma in the discharge tube. The value of the plasma frequency in this case is close to the resonant frequency of the dielectric ring. The observed scattering effect of an incident plane electromagnetic wave makes it possible to use this system as a key for controlling the transmission of electromagnetic energy at the frequency of the main magnetic resonance of the dielectric ring.

Influence of the non-uniform rf electromagnetic field on reproduction of electrical potential in plasma with magnetized electrons

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This work is dedicated to the study of the influence of the Gaponov–Miller gradient forces associated with non-uniform electric rf fields on the possibility of formation of the spatial distribution of electrostatic potential in the magnetic field in the plasma volume. The paper deals with the plasma characterized by following parameters: the temperature of electrons is about several eV, the temperature of ions is fractions of an eV, constant magnetic field is about 10^2–10^3 G, the frequency of the rf field that generates plasma is about 5 MHz. It has been shown using assessments and numerical modeling in the HELIC 1.0 software that the influence of the Gaponov–Miller forces can be manifested primarily as border effects near rf antennas. However, even for relatively large amplitudes of rf fields generated by an antenna (dozens of kV/m), potential wells of the Gaponov–Miller for electrons do not exceed 1 eV, and "hills" for ions are several eV. Thus, it has been demonstrated that the Gaponov–Miller gradient forces should be taken into account only as a clarifying, but not determining factor governing the possibility of creation electrical potentials about 10^2 V in the plasma.

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Numerical modeling of ns discharge development in strong magnetic field

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The numerical characterization of nanosecond pulsed discharges has been conducted in a strong magnetic field environment. Streamer discharge development and plasma generation in pure CO_2 was analyzed when magnetic field was directed along the axis of the discharge cell. Numerical simulations were based of a two-dimensional fluid model. It is shown that strong magnetic field affect dramatically on the plasma formation. The ns streamer diameter decreases significantly, plasma density increases. Calculations were carried out for different magnetic field values for fixed CO_2 pressure $P = 50$ Torr and fixed ns pulse voltage $U = 20$ kV. Streamer initiation and propagation was simulated on the basis of an axially symmetric two-dimensional fluid model. The system of equations under study consisted of transport equations for the densities of charged particles (electrons and positive and negative ions) and the Poisson equation for the electric field. It can be concluded that the streamer discharge sharply changes its characteristics with increasing magnetic field from $B = 0$ to 4 T for gas pressure 50 Torr. With a further increase in the magnetic field, the discharge parameters change much more smoothly. Thus, the reduced gyrofrequency $\omega/N = 4 \times 10^{-13}$ [rad m^3/s] (Hall parameter ~ 1) is an important threshold above which the transverse expansion of a pulsed nanosecond discharge in CO_2 can be practically neglected. This remark is very important when designing the electrodes of the supersonic magnetohydrodynamic channel, since an increase in the magnetic field above a certain value for each gas pressure allows one to avoid the development of a discharge in the boundary layers.

Recent results of hyperspectral diagnostics of a high-voltage spark with microstructured electrodes

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The results of complex registration of self-luminescence of the near-electrode region of the discharge simultaneously in several ranges of the spectrum from the near ultraviolet to the mid-ir (thermal) range are presented. The regions of primary ionization, regions of heating and expansion of the current channel, followed by dissipation of the deposited energy with a long relaxation phase are traced. Such "hyperspectral" imaging allows visualizing the primary streamer corona and the subsequent discharge channel even in difficult environmental conditions, such as a discharge in an aerosol cloud (including such a kind as a "stalker"), near-electrode regions with powerful plasma formation from the electrode material with the formation of microdroplets and metal vapor.

An intensified camera with a photocathode sensitive in the range of 180–800 nm is used in the uv and visible regions, a specially prepared CMOS (complementary metal–oxide–semiconductor) camera is used in the near-infrared region of 0.7–1.2 μm, and a thermal imaging camera with a microbolometric VOx matrix is used in the mid-ir region (5–12 μm, noise equivalent temperature difference NETD $<$ 40 mK) with a germanium lens.

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Study of the response of an optical system when registering a small-scale structure of an electric spark when probing with coherent light

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The work investigates the features of the image transmission of a fine-structured electric spark in an optical lens system, recorded using a probe laser radiation. The structure of such a spark is fundamentally small-scale, and the resulting laser shadow images and interferograms are partially distorted due to the influence of the instrumental function of the optical registration system. Here, we consider in detail probing of the fine-structured spark by 532 nm laser radiation. By simulating the spark image transmission in an optical registration system, we evaluate the effect of the system response function on the quality of the registered spark patterns. We show that the spark microstructure is reliably resolved only by optics having a spatial resolution better than several micrometers. Also, it is found out that the defocusing effect, which naturally arises due to the finite depth of field of an optical registration system, is crucial for precise investigation of complex-structured sparks and should be accounted for in the image processing. Our findings reveal extreme difficulties in diagnosing of the fine-structured spark and, at the same time, provide reliable basis for its comprehensive investigation.
The experimental part of the work is supported by the Russian Science Foundation (grant No. 19-79-30086). Theoretical analysis and data processing are founded by grants from the Russian Foundation for Basic Research (No. 20-08-01156) and the President of the Russian Federation (No. MK-703.2020.2).

Extraction of high-contrast diffraction patterns of fine-structured electrical sparks from laser shadow images

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A finely structured electric spark appears in a gas discharge in the form of a cluster involving dozens of closely-packed thin plasma filaments. To gain a deeper insight into the physics behind such spark, reliable data on its structure and characteristics of the transmitted radiation are of vital importance. However, immerse complicity of the spark, together with distortions and various defects of the optics involved in the laser imaging system, challenges the spark image processing. Herein, we present an iterative image denoising procedure for precise processing of shadow images of fine-structured sparks obtained by single-shot laser probing, implemented in a shadow photography system. By using the described procedure, we show that the passage of laser radiation through the fine-structured spark is accompanied by complicated diffraction, which, in turn, results in the high-contrast visualization of the spark microstructure in the entire discharge gap. The described procedure significantly advances processing of the laser shadow images of the fine-structured sparks as well as guarantees reliable quantitative data on the intensity characteristics of the transmitted laser radiation.
The experimental part of the work is supported by the Russian Science Foundation (grant No. 19-79-30086). Theoretical analysis and data processing are founded by grants from the Russian Foundation for Basic Research (No. 20-08-01156) and the President of the Russian Federation (No. MK-703.2020.2).

Interferometry in the study of the dynamics of a spark discharge in air in the point-plane gap

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It was found that the spark channel is a cluster of dozens of highly ionized filaments with a micron diameter and a subnanosecond evolution time, which is a promising option for the ignition of oxygen-depleted gaseous fuel due to rapid ionization in the discharge in the filamentation mode. These studies were based on the method of multi-frame laser sensing. The most important task in the experiments is the numerical processing of interferograms of axisymmetric plasma objects. Therefore, it is of great importance for our work to obtain a high-quality interference pattern, that is, the need to find the best type of interferometer for the task at hand and make a very precise adjustment. In this work, it was decided to use an interferometer with the use of an air wedge. A study was conducted of the interferometer of this type. Interference occurs as a result of the superposition of two laser beams reflected from the faces of an air wedge, which is located in the gap between two surfaces of glass 90-degree prisms pressed together. The width of the gap is adjusted by applying layers of adhesive tape. The study is supported by the Russian Science Foundation (grant No. 19-79-30086). Theoretical analysis and data processing are founded by the grants of the Russian Foundation for Basic Research (No. 20-08-01156) and the President of the Russian Federation (no. MK-703.2020.2).

Mean electric field and total near electrode drops measurements for discharge in hydrogen at initial pressure of 32 MPa with current amplitude of 1.3 MA

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Research results for discharge initiated by wire explosion in hydrogen at initial pressures of $\approx$ 32 MPa and current amplitudes of $\approx$ 1.3 MA between steel electrodes are presented. The new data enlarge the results of researches on this topic continuing from [1]. Mean electric field in discharge channel and mean near electrode voltage drops were determined in an experimental series with steel electrodes for different interelectrode gaps from 1 to 2 cm at the time of current maximum. The near electrode voltage drop was of $\approx$ 3.5 kV and electric field strength in the discharge channel was of $\approx$ 0.7 kV/cm at this conditions.

[1] Bogomaz A A, Budin A V, Pinchuk M E, Rutberg P G and Savvateev A F 2005 *Physics of Extreme States of Matter—2005* (Chernogolovka: IPCP RAS) pp 214–6

Gas temperature spatial distribution in air surface dielectric barrier discharge measured by schlieren imaging

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Spatial distributions of temperature of air in outer space near surface dielectric barrier discharge (SDBD) system are determined by schlieren technique. The diagnostic technique was considered methodically in [1]. High voltage electrodes consisted of ten parallel aluminum foil strips on one side dielectric barrier (1 mm thickness, Al_2O_3 or AlN), reverse electrode was grounded and covered all dielectric barrier plate side. The SDBD excited by sinusoidal voltage with root-mean-square value of 2–3.5 kV across the barrier of aluminum nitride with frequencies of ≈ 4 and 20 kHz were investigated.

[1] Pinchuk M E, Lazukin A V and Stepanova O M 2020 Air temperature spatial distribution in corona discharge with plane comb of metal rod electrodes obtained by schlieren technique *XXXV Int. Conf. on Equations of State for Matter. Book of Abstracts* (Elbrus) p 314

Simulation of plasma parameters of dc discharges at medium and high pressures within the kinetic approximation

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The paper presents a one-dimensional model of a direct current glow discharge at medium and high pressures in inert gases. The model includes the kinetic Boltzmann equation for the electron distribution function $f_0(x, w)$, taking into account the spatial derivatives both with respect to the coordinate and with respect to energy; block of continuity equations for ions and excited particles; Poisson's equation for a self-consistent field; equation of thermal conductivity to describe gas heating; equation for the external circuit. The collision integral of the kinetic equation includes elastic and inelastic processes (excitation, ionization, superelastic collisions), electron–electron collisions, and recombination. Preliminary numerical experiments have been carried out for such discharges with $pL = 3$ and 7 cm Torr at pressures from 10 to 150 Torr. This work was supported by the President's scholarship C-239.2021.1.

Numerical study of the dynamics of a surface barrier discharge in nitrogen

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A model of a surface dielectric barrier discharge in nitrogen is formulated in this work. The model is based on the continuity equations for charged, excited, and neutral particles, the Poisson equation for a self-consistent electric field. The equalization of the energy balance for the heavy plasma component and the vibrational temperature of nitrogen, as well as the Navier–Stokes system of equations for describing gas-dynamic effects in the discharge formation zone. In this work, numerical experiments are carried out for nanosecond barrier discharges. The parameters of the plasma in the active phase of the discharge and in the afterglow phase are determined. The influence of the "memory effect" during the formation of the discharge in the second pulse is determined.

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Plasma–liquid interaction during a pulsed vacuum breakdown

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The dynamics of phase changes in the material of a copper cathode during the explosion of a microprotrusion on its surface under the action of the explosive electron emission current has been numerically simulated. Numerical data have been obtained that characterize the interaction of the liquid metal and the dense cathode plasma that are formed due to the microprotrusion explosion. It has been shown that under the action of the pressure exerted by the plasma, the liquid metal is almost completely displaced from the zone of operation of the cathode spot of the vacuum discharge. This leads to the formation of a crater on the cathode surface with microirregularities at its edge. Thus conditions are created for the formation of new microprotrusions, which, when exploding, provide self-sustained and cyclic operation of the vacuum discharge.

Arc-plasma remelting of steel

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Low-temperature plasma is widely used in science and technology, in particular, for alloying steels with nitrogen during arc remelting, which is one of the most promising directions for creating high-strength, corrosion-resistant high-alloyed steels. The use of nitrogen in the gas phase makes it possible to obtain steel with a higher and more uniform nitrogen content, and the use of nitrogen plasma makes it possible to quickly obtain the required nitrogen content in the alloy due to the active absorption of nitrogen by the liquid metal, which exists in an excited and atomic state. To study the process of alloying steel with nitrogen, an experimental stand for plasma-arc remelting of steel was created, based on a vertically located low-temperature plasma generator with a direct arc. The physicochemical properties of both the plasma medium itself were determined (in the axial zone, the temperature and concentration of electrons 7000 K and 10^{16} cm^{-3}, respectively) as well as the properties of the resulting metal after remelting of steel grade 55Kh20G9N4. In which changes in the following properties were established: grain refinement, increase in strength, plasticity, total work of destruction, wear resistance under dry friction conditions and a decrease in the corrosion rate.

The present work was partially supported by the Russian Foundation for Basic Research (grants No. 19-08-0100 and 20-08-00224).

Investigation of the dependence of the structure of the discharge channel in a discharge with a liquid cathode from the electrochemical properties of a liquid cathode

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In the discharge with the liquid cathode, the discharge channel near the surface of the liquid cathode is divided into separate filaments. In this case, the filaments near the surface of the liquid cathode are in constant chaotic motion. Not only does their position in space and the size of the area they occupy change over time, but also their number. The influence of the specific electrical conductivity and pH of the solution on the position of the branch point of the discharge channel on individual filaments, the diameter of the filamentation zone near the surface of the solution, and the number of filaments in the liquid cathode discharge is studied. It is shown that as the specific electrical conductivity of the solution increases, the height of the filamentation zone, the diameter of the filamentation zone near the solution surface, and the average number of filaments fall. It is shown that for the same specific electrical conductivity of the solution, the maximum height of the filamentation zone, the minimum diameter of the filamentation zone, and the minimum average number of filaments are observed at a pH of the solution close to neutral.

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The analysis of electrical characteristics of the discharge with the liquid cathode with organic impurities

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The electrical characteristics of the discharge with the liquid cathode are studied. The role of the liquid cathode was performed by an aqueous solution with organic impurities. Various alcohols were used as organic impurities. The study was carried out for discharge chambers with different free surface areas of the liquid and different modes of mixing the solution near the liquid surface. In the discharge channel of the discharge with a liquid cathode, in the presence of various alcohols in the solution, the values of the field strength were determined. For this purpose, in each case, the dependence of the voltage drop on the discharge cell on the distance between the electrode and the solution surface at a given discharge current was constructed. Since this dependence is close to linear, the field strength in the discharge channel of the liquid cathode discharge was determined as the tangent of the angle of inclination of this line. It is established that the field strength within the error of determination does not depend on the presence and type of alcohol in the solution (at a concentration of up to 1% of alcohol by volume), as well as on the free surface area of the liquid in the discharge chamber, but depends on the mixing mode of the solution near the liquid surface. It is shown that the field strength in the discharge chamber (in the mode without mixing the solution) in all cases is 2.2–2.3 times higher than the field strength in the open air under the same conditions.

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

Application of gas chromatography to cold plasma jet analysis

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The prototype of a multipurpose microwave (2.45 GHz) plasmatron previously developed and manufactured for plasma surface modification makes it possible to generate atmospheric-pressure cold plasma jets by means of external portable plasma torch with a wide outlet of 2.5 cm in diameter and a microwave power of the order of several hundred watts. A microwave discharge is initiated when a plasma-forming gas flows through the torch. Discharge channels are formed between the rod electrodes and the inner wall of the cylindrical discharge chamber near the outlet of the torch. We have implemented a procedure for chromatographic analysis of the gas composition in microwave discharge zone inside the plasma torch and in a cold plasma jet that forms behind the outlet of the torch while interacting with atmospheric air. For the analysis of gaseous samples the chromatographic gas complex "Chromos GKh-1000" was used. Argon (99.993%) was supplied to the torch at a flow rate of 7.5 liters per minute The analysis of gas samples showed that new gaseous products (hydrogen and methane) are formed and the concentration of CO increases 5–6 times due to plasma–gas interaction. This effect is connected with increased mixing of atmospheric air containing water vapor to the argon flow in the discharge zone. The formation of carbon monoxide and hydrogen occurs in the processes of dissociation of CO_2 and the processes of direct decomposition of water vapor in a nonequilibrium plasma through vibrationally excited states.

This work was financially supported by the Russian Foundation for Basic Research under grant No. 19-08-00844.

Investigation of the effect of the electrochemical properties of the solution on the luminescence intensity of molecular nitrogen in a discharge with a liquid cathode

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For a discharge with a liquid cathode near the solution surface, the dependence of the radiation intensity of the second positive molecular nitrogen system on the discharge current at different conductivity and pH of the solution is found. It is shown that the radiation intensity of the second positive nitrogen system increases with a decrease in the conductivity and a decrease in the pH of the solution. For the discharge with the liquid cathode, the distributions of the luminescence intensity of the second positive system of molecular nitrogen in height are found for different electrochemical properties of the liquid cathode. It is shown that in all cases the intensity distribution over the height has two maxima. One near the metal anode, the other near the liquid cathode. Moreover, the maximum near the metal anode is approximately an order of magnitude higher in intensity than the maximum near the surface of the liquid cathode. It is shown that the vibrational and rotational temperatures determined from molecular nitrogen near the metal anode and liquid cathode do not depend on the electrochemical properties of the liquid cathode. The vibrational temperature near both electrodes was 3800 K. The rotational temperature near the metal anode was 1150 K, near the liquid cathode 2400 K.

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Energy conversion for plasma control of the lift force of an aircraft

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In the first part of this work, it was found that with a decrease in pressure and an increase in the length of the exposed electrodes, the efficiency of the "power source–actuator–dielectric barrier discharge (DBD)" system and its capacity significantly increase. This is accompanied by a decrease in the quality factor. The additional energy is spent primarily for producing and maintaining the synthetic jet. In the second part of the work, the lift force arising from the interaction of a synthetic jet with subsonic airflow at atmospheric pressure was measured. We used symmetric and double symmetric actuators, which were installed both on the lower surface of the profile and on the upper one. Pulsation of vortices in the region of interaction of a synthetic jet with an airflow at a frequency of 1–2 Hz was found. The synthetic jet, produced by the DBD, interacts with subsonic airflow and forms a long separation bubble. If the actuator is installed near the trailing edge of a symmetrical profile, then this bubble closes outside the wing, forming a "virtual" asymmetrical profile. An in-stream wing mounted actuator adds kinetic and thermal energy to the airflow. If the separated bubbles arising in this case are closed on the airfoil surface, we can speak of the effect of hypercirculation, which, in contrast to the classical blowing of jets onto the flaps, already has a minimum thrust for a continuous flow around. Consequently, any small effect of adding momentum to the flow will be more effective. For the full realization of this effect, the thrust of the synthetic jet may not reach large values, since an essential factor is the amount of energy transferred to the flow in relation to that spent on the generation of the discharge. With an increase in the surface area occupied by the discharge, the hypercirculation effect also increases.

Study of the interaction of helium plasma with tungsten divertor modules in the PLM plasma installation

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Computational modeling of plasma-facing material thermal loads of tokamak reactors including ITER is traditionally performed under assumption that the plasma transfer to the divertor plates and the first wall is ambipolar. However, using this assumption for estimating the heat load on the surface can yield underestimated values for heat flux on the divertor plates. Non-ambipolarity of the particle flux in tokamaks occurs at high values of radial electric fields, in regimes when accelerated electrons escape to the wall, as well as when electric arcs appear on material surface. Experimental studies of such processes with lower costs can be carried out on an experimental installation—a simulator of a divertor plasma, in which the following conditions are attainable: plasma stationarity, intense thermal loads on materials simulating loads at edge-localized modes, technologies for controlling parameters of the plasma-wall interaction. In Russia, MPEI has created such plasma stand—PLM (plasma linear multicasp).
This work was supported by the State Atomic Energy Corporation Rosatom, project EOTP-UTP-223; the study of the structure of materials was supported by grant No. 17-19-01469-P from the Russian Science Foundation.

Titanium oxide plasma melt

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At present, titanium oxide is used as a material for photocatalytic sterilization in the medical, food and mycobiological industries, as well as for solving environmental problems. The use of plasma technology to ensure high-quality melting of titanium oxide involves overcoming the full melting temperature (2116 K) and its subsequent rapid cooling. As a result, we can expect the formation of a vitrified state. An air high-voltage three-phase ac plasma torch was used in the experiment. The plasma torch was located on the top cover of the reactor. A water-cooled metal pipe was used to remove the waste plasma stream. The temperature on the surface of the melt was measured using a two-beam pyrometer. The composition and properties of the resulting sample were studied using a scanning electron microscope and an x-ray diffractometer.

Arc pyrolysis of methane in argon atmosphere

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Our team have developed a method for the synthesis of fullerene soot from hydrocarbons in an alternating current electric arc plasma torch. Depending on the hydrocarbon used, the content of light fullerenes in soot was from 1.5 to 7 percent by weight. Such a low yield is associated with the interaction of the synthesis products with hydrogen formed by pyrolysis. In order to remove this hydrogen, oxygen is supplied to the plasma torch. The plasma torch used consists of two perpendicular channels made of graphite. On three sides of these channels are graphite rod electrodes. The fourth side is the exit from the electric arc zone. Argon is supplied to the electrode area to prevent soot settling on fluoroplastic insulators. Methane is fed into the arc burning zone. The reaction products are cooled in a water cooler and collected in a cyclone. The resulting carbon black was analyzed by various physicochemical methods: scanning electron microscopy, photon correlation spectroscopy, electron spectroscopy of the extract. Carbon amount varies from 89 to 97 percents. There is oxygen everywhere (from atmosphere).

Fullerenes production by electric arc pyrolysis of methane in a three-phase ac plasma torch

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The present work deals with a high-voltage three-phase ac plasma torch working as a part of a plasma-chemical facility. This plasma torch consists of three electric arc channels and three rod copper electrodes. The initial breakdown occurs with high voltage (10 kV) provided by a high voltage power supply. The electric arc plasma oxygen-free pyrolysis of methane was realized on the facility. The fullerene-containing fraction was extracted from the carbonaceous material by extraction with ortho-xylene. Nanocarbon material with submicron particle sizes was produced by the method of oxygen-free electrical arc pyrolysis of methane. The resulting carbon black contained particles of graphite (66%) and amorphous carbon (34%), as well as light fullerenes in amounts up to 3%. Infrared spectroscopy showed reflexes typical of C–C bonds in graphite and C–H in polynuclear hydrocarbons. The spectrum is characterized by some peaks in the near uv region, in particular, $\lambda = 337 \pm 2$ nm, characteristic of light fullerenes. X-ray diffractometry showed the presence of graphite and amorphous carbon. On these grounds it can be assumed that this method can be applied as a low-cost and effective method for the synthesis of fullerenes.

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