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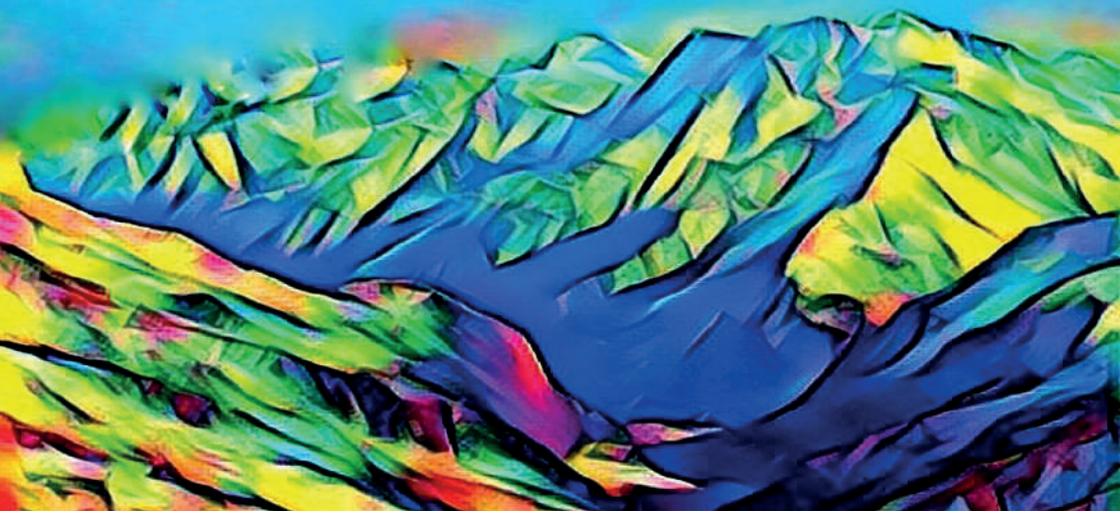


XXXIII International Conference on Equations of State for Matter

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The book consists of abstracts of plenary lectures, oral reports and posters presented at the XXXIII International Conference on Equations of State for Matter (1–6 March 2018, Elbrus and Tegenekli, Kabardino-Balkaria, Russia). The conference is devoted to the 40th anniversary of the I All-Union Session on Equations of State (October 1978). The presentations deal with the contemporary investigations in the field of physics of extreme states of matter. The conference topics are as follows: equations of state and constitutive equations for matter at high pressures and temperatures; shock waves, detonation and combustion physics; interaction of intense laser, x-ray and microwave radiation, powerful ion and electron beams with matter; techniques of intense energy fluxes generation; experimental methods of diagnostics of ultrafast processes; low-temperature plasma physics; physical issues of power engineering and technology aspects.

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The editorial board with deep regret announces the death of friends and colleagues: Academician Evgeny Nikolaevich Avrorin (11 July 1932 – 9 January 2018), who was the organizing committee member of the Conferences on Equations of State for Matter and Interaction of Intense Energy Fluxes with Matter; Professor Valentin Fedorovich Kuropatenko (18 December 1933 – 13 October 2017), who was an active participant in these meetings starting with the first session; Professor Mikhail Fedorovich Ivanov (29 September 1945 – 16 October 2017), who was a regular participant of these conferences too.

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Chapter 4. Physics of Low Temperature

Plasma

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1. Equations of State for Matter

Is there chemistry at megabars?

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Methods and some results of study of physical-chemical processes in materials in shock waves are discussed.

Phase transitions in silicon at high pressures and temperatures

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Thermodynamic model of equation of state and phase transitions of Si is necessary for numerical simulations of hydrodynamic processes in this material under intense pulsed influences. In the present work, a semiempirical approach is used for constructing the thermodynamic potential Helmholtz free energy for silicon with taking into account polymorphic transformations, melting and evaporation effects. The multiphase equation of state is built, and calculations of parameters of the phase diagram in a wide range of densities and temperatures are carried out. A comparison of calculated results with available data from static and dynamic experiments with Si at high energy densities is made.

Relativistic effects analysis of the electron binding energies in many-electron atoms

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The method of simultaneous analysis and presentation of the data on $\{E_{nl}^{(Z)}\}$ in a large number of atoms is proposed based on the atomic number scaling showed in [1, 2]. The scaling makes it possible to reduce the description of the whole data in any number of elements to the two functions $e_n(\sigma_n)$ and $d_n(\sigma_n)$. Here $\sigma_n = \pi n Z^{-1/3}$, and the corresponding values e_n and d_n are calculated using the equations $e_n = E_{n0}/Z^{4/3}$ and $d_n = (E_{nl} - E_{n0})/Z^{2/3}\lambda^2$. The pairs of numbers $e_n - \sigma_n$ for all the atoms ($10 \leq Z \leq 92$) and all the numbers n form approximate common dependence $e(\sigma)$ in the closed energy shells ($\sigma_n \leq 3.3$), the relativistic effects little affecting this dependence, without changing its single-valued monotonically diminishing nature. If the relativistic effects are small, i.e. for the elements $10 \leq Z \leq 40$ the function $d(\sigma)$ behaves similarly. However, in the heavy atoms the single-valued nature of function $d(\sigma)$ is lost: the visible d_{nl} -branching for the different l , and in addition, a bifurcation due to the spin-orbit interaction for each l occur. Here an increase in the relativistic effects with an increase in the atomic number is visually manifested, all the dependence on σ preserving smooth nature and fitting the corresponding dependence for the inert gases. This can be used, for example, for the new data verification and for the recovery of the missing information about the binding energies in the neighboring atoms.

- [1] Shpatakovskaya G V and Karpov V Ya 2016 *J. Phys.: Conf. Ser.* **774** 012002
- [2] Karpov V Ya and Shpatakovskaya G V 2017 *J. Exp. Theor. Phys.* **124** 369

Melting T – P curves for alkali metals with negative slope and minimum: Electronic origin

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Group I elements—alkali metals from Li to Cs—are examples of simple metals with $1s$ electron in the valence band. Under pressure they display unusually complex structural behavior transforming from close-packed to low symmetry open structures. Unexpectedly complex form was found for melting curves of alkalis under compression with initial increasing in accordance to Lindemann criterion and further decreasing to very low melting point [1,2]. To explain complex and low symmetry structures in compressed alkalis the model of the Fermi sphere–Brillouin zone interaction was applied [3,4]. Within this model one can understand the complex melting curves of alkalis. Deep minimum on melting curves is related to overlap of valence electron band and core electrons similar to suggested transfer for the structures Na- $oP8$ and K- $oP8$ assuming that Na and K become divalent metals at compression. Electron transfer may occur in liquid state and even at lower pressure. Non-simple behavior in melting of alkali metals on compression is connected with the essential changes of the electron state in the valence band [5].

- [1] Gregoryanz E, Degtyareva O, Somayazulu M, Hemley R J and Mao H k 2005 *Phys. Rev. Lett.* **94** 185502
- [2] Guillaume C L, Gregoryanz E, Degtyareva O, McMahon M I, Hanfland M, Evans S, Guthrie M, Sinogeikin S V and Mao H K 2011 *Nat. Phys.* **7** 211–214
- [3] Degtyareva V F and Degtyareva O 2009 *New J. Phys.* **11** 063037
- [4] Degtyareva V F 2014 *Solid State Sci.* **36** 62–72
- [5] Degtyareva V F 2017 *Cogent Phys.* **4** 1327697

Verification of anomalous thermodynamic properties of sodium near its melting curve

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Using the classical molecular dynamics method Belashchenko [1] revealed a region of anomalous thermodynamic properties of sodium near its melting curve. He used an embedded-atom model for liquid metal and fitted free parameters of the potential to structural data at 378, 473 and 723 K as well as to thermodynamic properties of sodium at pressures up to 96 GPa. It was found the region with a negative isochoric pressure coefficient $1/P(\partial P/\partial T)_V$; this means that some other coefficients such as Grüneisen parameter and adiabatic thermal expansion coefficient are also negative. The anomalous thermodynamics region is close to the experimental melting curve [2] and is connected with the formation of clusters of sodium atoms. We recalculate the same isochors using quantum molecular dynamics and do not confirm any thermodynamic anomalies: the slope of the isochors is always positive in temperature–pressure coordinates. This work has been done under Russian Foundation for Basic Research financial support, grant No. 17-08-00736.

[1] Belashchenko D K 2009 *High Temp.* **47** 494–507

[2] Gregoryanz E, Degtyareva O, Somayazulu M, Hemley R J and Mao H 2005 *Phys. Rev. Lett.* **94** 185502

Wide-range equation of state for gold

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Results of theoretical calculations and experimental measurements of the equation of state (EOS) are discussed and applied to gold. The thermodynamic properties of gold and its phase diagram are calculated with the use of multi-phase EOS model. Theoretical calculations of thermodynamic properties of the solid, liquid, and plasma phases, and of the critical point, are compared with results of experiments. The analysis deals with thermodynamic properties of solid metal at $T = 0$ and 298 K from different band-structure theories, static compression experiments in diamond anvil cells, and the information obtained in shock-wave experiments. Thermodynamic data in the liquid and plasma states, resulting from traditional thermophysical measurements, “exploding wire” experiments, evaluations of the critical point and measurements of the principal Hugoniot are presented. These data are analyzed in a self-consistent manner.

Thermodynamic properties of hydrogen and helium in megabar pressure range

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The thermodynamic properties of hydrogen and helium at high pressures and temperatures are of interest for many years because of their wide spreading in the universe. At these parameters a high density of matter is accompanied by a strong Coulomb interaction (strongly non-ideal plasma). In spite of achievements of experimental and theoretical methods in this range of parameters further study of dynamically compressed hydrogen and helium is important. In particular, the problem of the possibility of a phase transitions at high compression degrees is not resolved yet. Last several years new theoretic results in frames of chemical picture and ab-initio methods in a wide range of pressures generated with shock and quasiisentropic compression have been presented. Here we present the results of calculation of equation of state of hydrogen and helium along principal Hugoniot and isentropes. These calculations were carried out with codes implemented the improved SAHA-family models. The thermodynamic properties of hydrogen and helium up to several terapascal and high temperatures are presented. The calculations have shown that in the considered pressure range dynamically compressed hydrogen and helium is in a state of strongly coupled, degenerated plasma with density close to condensed matter. Results of our calculations are discussed together with those obtained in frames of the first principal quantum methods and the data of new experiments.

Anomalous thermodynamics and entropic fluid–fluid phase transition problem in highly compressed hydrogen and nitrogen

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Anomalous properties of adiabatically compressed molecular gases in megabar pressure range may be realized due to existing of anomalous thermodynamic (AT) properties of warm dense hydrogen (deuterium) or nitrogen in extended region of their phase diagram. Such AT region always accompanies the so-called entropic 1st-order delocalization-driven fluid–fluid phase transition [1]. The main feature of AT region is simultaneous loss of positivity by great number of 2nd-order cross derivatives for thermodynamic potential, such as Grüneisen parameter, thermal expansion coefficient etc (see e.g. [2,3]). One of the main manifestation of AT are mutual crossing and disorderliness of many isolines, e.g. isotherms, isoentropes, Hugoniot etc. The discussed anomalies lead in turn to corresponding hydrodynamics anomalies in compression and expansion adiabatic flows. Mentioned above anomalies in pure planetary gases (hydrogen, helium, nitrogen etc) became much more complicated due to additional appearance of non-congruence for all phase transformations in the case of mixed planetary materials, such as the hydrogen–helium–water–methane–ammonia mixture.

[1] Iosilevskiy I L 2015 *J. Phys.: Conf. Ser.* **653** 012077

[2] Iosilevskiy I L 2013–2017 *Scientific-Coordination Session on Non-Ideal Plasma Physics* (Moscow)

[3] Iosilevskiy I L 2015 *XXX Int. Conf. on Interaction of Intense Energy Fluxes with Matter. Book of Abstracts* (Nalchik: IPC KBSU) pp 146–147

Interpretation of experimental data scatter for the fluid–fluid phase transition in hydrogen

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Supposition is made that metastable states formation is a reason of the shift of Z-machine and National Ignition Facility results with respect to the diamond-anvil-cell (DAC) and shock-wave results. It is an effect of different compression or heating rates. The faster is the compression or heating rate the farther from the equilibrium transition and closer to the spinodal is the point of the experimental transition. In this case, both Marcus Knudson (SNL), and Peter Celliers (LLNL), and DAC (Harvard and Japan), and shock-wave (Sarov and JIHT RAS) people could be right. The abstract was prepared within the framework of the basic research program at the National Research University Higher School of Economics (HSE) and supported within the framework of a subsidy by the Russian Academic Excellence Project “5-100”.

Mechanism of the transition to the conducting state in solid hydrogen at high pressures

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The mechanism of the phase transition of solid hydrogen (or deuterium) to the conducting state is suggested. Within the framework of the density functional theory The dependencies of the pressure, electrical conductivity and profiles of the proton-proton pair correlation function (PCF) of hydrogen on the density and at temperatures 100 and 50 K have been calculated. The considered density range $\rho = 1.0\text{--}3.0\text{ g/cm}^3$, the calculated pressure range is 300–1000 GPa, which corresponds to the solid phase of hydrogen. A pseudopotential approach is used to describe internal electron shells (core electrons), in particular, the nonlocal potential of projector augmented waves (PAW) is used. For valence electrons, the Kohn–Sham system of equations with the PAW potential is solved. Structural transition occurs, characterized by the appearance of the first peak of the PCF at a distance of 0.92, which corresponds to the interatomic distance in the H_3^+ ion. Thus, the nature of the transition combines ionization with structural changes. With further compression, the first maximum of the PCF corresponds to the average distance between the particles at a given density, which indicates the complete dissociation of hydrogen ions. Strong ionization during the phase transition in dense solid hydrogen (or deuterium) brings this transition closer to the prediction of the Norman–Starostin plasma phase transition. The study has been prepared within the framework of the basic research program at Higher School of Economics and supported within the framework of a subsidy by the Russian Academic Excellence Project “5-100”.

Metastable states of warm dense hydrogen

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Warm dense hydrogen is investigated by ab initio molecular dynamics simulations in the region of fluid–fluid phase transition. The simulation is made in the framework of density functional theory. The supercell contains 512 atoms, time step is 0.5 fs. The hydrogen is observed along 700 and 1000 K isotherm at the density interval of 0.88–1.94 g/cm³. The Perdew, Burke and Ernzerhof (PBE) functional is used, since it reproduces experimental pressures and temperatures of phase transition. Modeling of metastable states is an unexplored problem so far. There are two main points that let us to obtain the metastability: the selection of particular initial configurations (coordinates and velocities of ions) and turning off the thermostat. We managed to obtain molecular phase far beyond the phase transition. The metastable branch of the isotherm overlaps the equilibrium branch by density at the interval of 0.09 g/cm³ for 700 K and 0.05 g/cm³ for 1000 K, that is several times more than density jump at the phase transition. The pressure range of metastability studied is more than 300 kbar for both temperatures, while the difference between pressure of the metastable and equilibrium states at the same density is approximately 150 kbar. The pair correlation function conserves its shape along the isotherms, that confirms the preservation of the molecular phase. The work is supported by the Russian Science Foundation (grant No. 14-50-00124).

Brightness temperature and electric conductivity of multiple shocked initially gaseous deuterium and helium up to 0.4 TPa

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Deuterium or helium sample at initial temperature of 78 K and pressure 10–27 MPa, was multiple shock compressed between dielectric sapphire window and brass or sapphire driver plate; high pressure pulse was provided by conical Mach generator of shock wave. Brightness temperature of compressed sample was registered, along with its reflectivity at 807 nm pyrometer channel. Electrical resistance of the compressed sample layer was measured by three or four electrode constant current measuring circuit, depending on driver plate material. Process of compression was simulated by 1D and 2D hydrodynamic codes with use of wide-range semiempirical equation of state (EOS) of sample and assembly materials. Results of measurements were compared with simulation results, utilizing two hydrogen EOS models—SESAME and model with proposed metal–insulator transition.

Evaluation of the critical point parameters of liquid–vapor transition of boron

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The expanded final states with pressures 0.004–1.55 GPa of initially porous ($m = 5\text{--}6$) boron (amorphous form) from a shock compressed state with pressures of about 20 and 30 GPa were studied by optical pyrometry. The heating of the sample surface layer in the process of expansion were observed. The fast heating and evaporation of the boron particles in shock-compressed helium at particle velocity 6–12 km/s was registered. The position of the critical point of liquid–gas transition in p – T coordinates for boron was determined as $p = 1.25$ GPa, $T = 8500$ K with error bars estimated as 0.2 GPa and 300 K. This position is close to prediction of A A Leont'ev, A N Dremin and V E Fortov (1978): 0.957 GPa and 8200 K.

Critical temperatures of alkali metals: Estimated calculations

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There is little reliable information in the literature on the critical temperature T_c of metallic melts, including alkali metals [1, 2]. In the present paper, the task is set to further refine T_c of alkali metals, taking into account the new experimental data on the temperature dependence of the surface tension $\sigma(T)$ (ST) of alkali metals. In order to calculate T_c , we used the fact that, at a critical temperature, the ST of the substance vanishes. Therefore, having data on $\sigma(T)$ of a metal or an alloy, we can estimate T_c from the ratio

$$\sigma(T) = \sigma_m - \frac{\partial\sigma}{\partial T}(T_c - T_m).$$

We only note that the assumption that the $\sigma(T)$ curve is linear in the entire region of existence of the liquid state of the metal or alloy is the main source of the error in determining the value of T_c , but on the other hand, most close to the critical temperature range [3]. Using the precision data about ST on the alkali metal obtained on high purity samples and ultrahigh vacuum conditions, critical temperatures of alkali metals have been calculated in this paper. It is shown that calculated values of critical temperatures of the specified metals well will be coordinated with results of theoretical calculations available in literature and pilot studies.

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Thermodynamic parameters and electrical conductivity of copper in the near-critical region of the liquid–vapor phase transition

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Study of thermodynamic parameters of copper in near-critical region of liquid–vapor phase transition and the predicted metal–nonmetal transition was carried out. The measurements of electrical conductivity of copper after shock compression and expansion in gas (helium) medium at different final pressure were carried out. It was discovered, registration of time dependence of electrical resistivity of the expanded metal has allowed to estimate their density in the near-critical point region of liquid–vapor phase transition. Hydrodynamic simulation of the process of shock compression and expansion of the copper at the experiments on shock compression and expansion of copper in gas medium was made. Simulation allows us to estimate the density gradient of the sample and to choose the position of the pin-electrodes at the assembly when the density gradient is minimal.

Electrical resistivity of liquid expanded metals by Ziman approach

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Transport properties of metals near the critical points were intensively studied [1, 2]. Using quantum dynamics simulations, we consider the structures of liquid aluminum and copper at high equilibrium temperatures and strong compression. On the other hand, we carry out classical molecular dynamics (MD) simulations using the embedded-atom method (EAM) interatomic potentials. Both approaches provide data for resistivity calculations based on the well-known Ziman–Evans (ZE) formula. The results of these calculations show a weak dependence on the used methods of ion structure computations. Also, we demonstrate that an effect of electron temperature, which is implemented in the effective electron–ion potential used in the ZE formula, is negligible at electron temperatures less than 30 000 K. This work has been supported by Russian Science Foundation (grant No. 14-19-01599).

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Equation of state of fluid aluminum in the metal–nonmetal transition range

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A phenomenological equation of state has been constructed for Al to study thermodynamic consequences of the metal–nonmetal transition occurring in this fluid. Based on the experimental fact that isochores plotted in the internal energy–pressure plane are straight lines it is shown that the equation of state must have the Mie–Grüneisen–Debye form, so that the cold curve, the Grüneisen coefficient, and the Debye temperature retain certain physical significance for the fluid. These characteristics have been determined for a wide density range and compared with the literature data.

Heat transfer in supercritical region: The problem of reconciling results of pulse and stationary experiments

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Our report is devoted to non-stationary heat transfer in supercritical region at small time and spatial scales. The aim of this study was to clarify the characteristic features of heat conduction mechanism at significant heat loads. For this purpose, the method of controlled pulse heating of fast-response wire probe was used. The characteristic heating time was a few milliseconds, and the heat flux density through the probe surface was increased up to 20 MW/m². The experimental values were obtained by direct processing of primary data and do not contain model constraints. The most important results obtained at small characteristic sizes and times can be formulated as follows. For all substances studied, the threshold decrease in the heat transfer intensity has been revealed in the course of a fast transition between compressed liquid and supercritical fluid states along the isobar. This effect was more pronounced, the closer was the pressure value (p) to the critical pressure (p_c). The effect was observed over a wide range of reduced pressures, up to $3p/p_c$. It was found that the peaks of isobaric heat capacity and excess thermal conductivity, which are known from stationary measurements, do not affect the experimental results. The discussion of the problem of reconciling our result with the peaks of thermophysical properties, which are known from stationary experiments in the near-critical region, appeared to be timely. Such situations are occasionally encountered in experimental thermophysics (and not only in it). A constructive approach for resolving this contradiction is to adapt fast-acting methods based on micro-sized heaters to the conditions of the problem under discussion.

Carbon in the megabar pressure range: New experiment and calculations

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The properties of carbon at high pressures and high temperatures are a subject of interest for many branches of science, including astrophysics and planetology, material science, applied engineering, etc [1, 2]. In this context, we performed an experiment addressed the study of equation of state and phase transitions of carbon at megabar pressures, using the PHELIX laser beam to generate a planar shock as well as two VISARs and target-rear-side self-emission diagnostics, both time-resolved by using streak cameras. As targets, we used diamond monocrystals with a plastic layer used as ablator and some metallic layer to provide the measurements of shock velocity. Due to the large thickness of the targets, the shock is expected to decay as it propagates due to 2D effects. To analyze data, 1D and 2D numerical simulations were realized. The results are discussed.

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Thermodynamic parameters of lithium deuteride in pressure ranges 5–1000 GPa

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The results of numerical experiments on modeling of shock-wave loading of lithium deuteride using the thermodynamic equilibrium model of thermodynamic equilibrium components (TEC) are presented [1, 2]. It is well known, that compounds of lithium with hydrogen are of interest as applied and fundamental points of view. Extensive scientific literature, in which a considerable part is occupied by researches with high impact and static pressures, is devoted to the research of thermos-physical properties of these compounds. However, the relatively low values of pressures up to 100 GPa are investigated in most of these works. The developed model allows us to describe thermodynamic parameters hydrides of lithium of different porosity, in a wide range of pressure values using model ratios, the experimental and theoretical data describing thermodynamic properties of the hydrides of lithium. Comparison of the model calculations with experimental data and calculations by other models confirms the validity and acceptable accuracy of the used model equations. The parameters of the equation of state can be used for calculations of thermodynamic parameters as for the pure LiD and mixtures and alloys comprising LiD in its composition, as relatively low pressures and temperatures and in high pressures, temperatures and densities, the condition in which is can be judged only by theoretical models [3].

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Theoretical investigation of the relative compressibility of metals in strong shock waves

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In this report, equations of state (EOSs) for aluminum, copper, iron, molybdenum and lead are constructed by the Thomas–Fermi model with corrections [1] and Hartree–Fock–Slater model [2] with different ways to take into account the ionic subsystem contribution [3]. The EOSs are used to derive the shock adiabats of substances in question. Calculation of shock adiabats is a convenient approach to investigate these EOS models, because experimental data are available on the compressibility of several materials in strong shock waves, where the temperature and density are sufficiently high to apply the quantum-statistical approximations. Moreover, the shock adiabats express the thermodynamic properties of matter in the form of a simple kinematic dependence $D(U)$, where U is the mass velocity, D is the shock-wave velocity. An analysis of the results of experiments on the relative compressibility of aluminum and copper in strong shock waves was carried out. Iron, molybdenum and lead were chosen as reference substances.

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Ion-correlation average-atom model in the limit of weak non-ideality

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Using the average-atom model of Starrett and Saumon [1] that allows for ion correlations, we have examined interionic potentials, pair correlation functions, ionization-potential depression, thermodynamic functions, and electron transport properties in the high-temperature and low-density limit. Unlike commonly used average-atom models disregarding ion correlations, the Starrett and Saumon model does provide the correct Debye–Hückel limit of interionic potentials, pair correlation functions, ionization-potential depression, and electron transport properties. The Coulomb logarithm in the asymptotic expressions of the transport coefficients obtained depends on the geometric average of electron and total (due to both electron and ion screening) Debye radii. The asymptotics of thermodynamic functions are essentially conditioned by the definition of the central-atom contribution to the total free energy of the infinite system of charged particles considered in the Starrett and Saumon model.

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Pseudo-atom molecular dynamics for the equation of state and ionic microstructure applications

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We present an implementation of pseudo-atom molecular dynamics (PAMD) simulation model [1, 2] for calculation warm and hot dense matter (WDM) thermophysical properties. Realistically description of ion-correlative effects and other Coulombic features can be taken into account in several ways indeed. Specifically, we can construct an effective interionic potential V_{II} in the first approximation as it has done in the model by C. E. Starrett and D. Saumon [3]. This potential may be used in the Ornstein–Zernike (OZ) set of equations iterative solver for self-consistent radial distribution functions (RDFs) obtaining. But in some extremely non-ideal cases we may characterize an ion microstructure with the help of classical MD modeling only. We present WDM as a set of neutral pseudoatoms and electrons, obtain spatial configurations of ions interacting via V_{II} , and directly finding ion-correlative energy terms. As in our previous reports, electronic subsystem in plasmas is considered in semiclassical way in the Thomas–Fermi–Dirac approximation. We compare the WDM equation of state obtained with PAMD method with results of the Helmholtz free energy differentiation in OZ-like model and determine the area of applicability for the last one.

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Equations of state for a condensed medium with a high energy density in a quasiclassical model

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In the semiclassical approximation, the equation of state of a perturbed condensed medium with a high energy density is studied. Accurate implementation of the model proposed in this paper complicates the calculation process. The theory of an inhomogeneous electron gas (the density functional theory) continues to develop and be used in various fields of physics. In this paper, we calculate the static perturbation of a condensed medium in the Thomas–Fermi model approximation with corrections for the inhomogeneity of the electron distribution. In [1], the necessity of solving this problem arose in calculating the polarizability of atoms, namely, when choosing a trial function in the variational approach. In this case, it was found necessary to take into account the gradient corrections in describing the properties of a substance with a high energy density. Problems for the electronic component for the spherically symmetric case are solved. The obtained result is in good agreement with the qualitative estimates obtained earlier in [1] for weak fields and the results given in [2]. This work was supported in the framework of the base part of the Minobrnauka task Kabardino-Balkarian State University for years 2017–2019 (project number 3.8382.2017).

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Advantages and limitations of average atom models at the development of wide-range equations of state

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In the last decade dominating approaches for ab-initio simulations of matter are based on the density functional theory (DFT) [1]. A limited subsystem of atoms is placed in a box with periodic boundary conditions where the self-consistent field and electron wave functions may be calculated at given density and temperature. Thus, Kohn-Sham DFT may provide the required amount of occupied electron energy levels for the proper calculation of thermodynamic functions. However, the approach is limited by the quite high temperatures of about tens of eV where it becomes impossible to account the all occupied levels. Orbital-free DFT can deal with that by the price of excluding discrete electron states what also removes shell effects [2]. Using the most simple DFT case (the Thomas–Fermi atom), we demonstrate that discrete and continuous representations of electron states may be linked providing proper thermodynamics with shell effects for warm dense matter and rarefied plasma [3]. The low-temperature limitations of our approach are discussed.

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First-principle study of critical parameters of tungsten

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We present quantum molecular dynamics calculations of thermodynamic properties of expanded liquid tungsten. We reproduce various shock-compression experiments for porous tungsten and subsequent isentropic expansion into different obstacles. Special attention is paid to available isobaric expansion experimental data and theoretical estimations of critical points. Density on our first-principle isobar of liquid tungsten is slightly higher than in most wire-explosion experiments and the slope of the isobar is more flat. A special Monte Carlo analysis has been applied for the estimation of the liquid–gas coexistence curve and critical point parameters of tungsten. The result is close to an estimation obtained with Likalter’s similarity relation.

Investigation of chemical bonds evolution in NiAl systems by ab-initio and classical molecular dynamics

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High-density reactive materials (HDRM) can be used for a rapid exothermic reaction under a mechanical or thermal action and high temperature without a significant increase in volume and formation of gas products. The Ni–Al system is an important subclass of HDRM. It is interesting to calculate chemical and physical behavior of the material during the reaction involving diffusion, heating, structural changes and phase transitions. Atomistic modeling can provide detailed fundamental information about reactive Ni–Al systems using empirical computational models or the classical molecular dynamics (MD) method using interatomic potentials of the embedded atom model (EAM). This paper presents an analysis of the lifetime of chemical bonds in a Ni–Al melt as a function of temperature and pressure, and compares this parameter for the methods of quantum and classical molecular dynamics. Modeling by the classical MD method is carried out using the LAMMPS package, the interaction between the particles is described using the interatomic potentials proposed in [1]. To demonstrate the applicability of the classical potentials under compression we calculate the cold curves of Ni, Al, and NiAl. The lifetime of chemical bonds is estimated using the analysis of MD configurations. The quantum MD method is realized by means of the computational package VASP, based on the density functional method.

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Soft-sphere model for entropy estimation in molecular dynamics

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Soft-sphere and hard-sphere models are widely used to simulate different properties of complex systems. For example, the hard-sphere potential is used to construct a perturbation theory in simple liquids [1] and for approximate simulation of entropy in a two-phase thermodynamic (2PT) model [2]. In this model it is able to estimate entropy of a system using only a single computer run. In the model entropy of liquid is a sum of entropies of solid and gas subsystems. For the gas subsystem the hard-sphere model is used to represent the tail of the velocity autocorrelation function (VACF) frequency spectrum; as the agreement is often unsatisfactory memory functions are applied to improve the situation. Nevertheless in many cases it is impossible to describe the gas part of the VACF frequency spectrum correctly. In this work we apply the soft-sphere model instead of the hard-sphere one [3]. It is known that a system with the soft-sphere potential has self-similar thermodynamic and dynamic properties owing to the homogeneity of the potential [4]. We present some results of molecular dynamic simulation of thermodynamic properties, self-diffusion coefficient, VACF for a soft-sphere gas. The analysis of entropy reconstruction from VACF will be also discussed.

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On consistency of dynamic experiments on thermodynamic properties of expanded liquid molybdenum

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In this work we present an analysis of isobaric expansion data for the liquid molybdenum. *Ab initio* calculations are used for comparison with experimental data on shock compression, isentropic expansion and isobaric expansion of liquid metals. Data for comparison includes results of static and dynamic experiments and multi-phase equation of state in view of the discrepancy between the experimental results obtained by different experimental groups.

Molecular dynamic simulation of isentropic expansion of aluminum into liquid–gas two-phase region

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Isentropic expansion is a useful tool for investigation of thermodynamic properties of expanded metals at high temperatures. This is one of a few techniques which can be applied to reach near-critical states of most metals. For refractory metals, i.e. molybdenum and tungsten, isentropes with initial points on a porous shock Hugoniot may penetrate into the liquid–gas two-phase region [1]. This effect is accompanied by the break on the experimental isentrope due to the sharp drop of sound velocity in the two-phase region. However, the true reason of the break is still unclear as the process of homogeneous nucleation should be taken into account in metastable regions; also the position of the boundary of the two-phase region for refractory metals is currently unknown. In this work we use molecular dynamics to simulate the effect of penetration of a release isentrope into the two-phase region by example of aluminum. This metal is chosen because there is a good-quality potential for aluminum with a known boundary of the liquid–gas two-phase region [2]. First results of aluminum release into argon of different initial pressure will be presented.

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Calculation of adiabatic expansion of nonequilibrium steam-drop media

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Nonequilibrium arises in many almost important problems of non-stationary gas dynamics. In particular metastable states are formed at fast expansion of metals vapors [1]. Transition to area of two-phase states is caused by faster decrease of temperature at adiabatic expansion in comparison with dependence of temperature of saturated steam on specific volume. Nucleuses number evolution is described by analogy with gases kinetic theory. In the issue we have infinite system of ordinary different equations. Using of continuous function of nucleuses size distribution leads to Fokker–Plank equation (it is named Frenkel–Zeldovich equation in [2, 3] if we consider nucleation problem). It is known that nucleation problem solution [4] included quasi-equilibrium distribution for nucleuses of prestalling sizes is applied for long processes. The system of ordinary different equations and Fokker–Plank equation are solved by numerical methods. Using of implicit finite-difference schemes allows reaching of quasi-stationary nucleation regimes. Fokker–Plank equation is used at a large number of the atoms which are contained in a drop. Such approach gives the possibility for consideration of finite number of the equations entering in kinetic system. Settlement results of adiabatic curves of metals vapors are given for various speeds of expansion. Work is made with support from the Russian Foundation for Basic Research (project 16-08-01065).

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Analytical approximation to equation of state for degenerate electron gas

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The degeneracy of electrons in a rather dense plasma results in the increase of its pressure, with the equation of state to be appreciably modified. The energy spectrum of degenerate electrons is presented by the Fermi–Dirac distribution; the density of electrons n , and their pressure p as well, can be expressed in the implicit integral formulas through the temperature T and chemical potential μ [1]. There appears a key dimensionless parameter in the problem, the degeneracy parameter $A = n(2\pi\hbar^2/mT)^{3/2}$, where m is the electron mass, \hbar is the Planck constant; this parameter A is related to the Fermi energy ε_F , $A = (8/3\sqrt{\pi})(\varepsilon_F/T)^{3/2}$. Due to analytical expansions one can obtain the equation of state for degenerate electron gas in an explicit form, with its extreme cases being as follows:

- (i) weakly degenerate electron gas, $A \ll 1$, $p/nT = 1 + A/8\sqrt{2}$;
- (ii) strongly degenerate electron gas, $A \gg 1$, $p/nT = (0.1\sqrt[3]{9\pi})A^{2/3} + 2(\pi/3)^{5/3}A^{-2/3}$.

So that to confirm the analytical approximations obtained, a direct computer calculation is performed with the exact integral formulas of the Fermi–Dirac distribution over the range $10^{-2} < A < 10^2$. These approximations prove to be decent matching the calculation over the whole range of parameter A , including the mid area $A \sim 1$. Thus the equation of state for degenerate electron gas takes a clear representation through the unique degeneracy parameter A and looks suitable at a wide density–temperature range.

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Anomalies of spatial ions distribution in trap in local equation of state approximation

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Impressive appearance of discontinuities in equilibrium spatial charge profiles in non-uniform Coulomb systems is under discussions in wide number of thermo-electrostatics problems. Such discontinuities are considered as peculiar micro-level manifestation of phase transitions and of intrinsic macro-level non-ideality effects in local equation of state (EOS), which should be used for description of non-ideal ionic subsystem in frames of local-density approximation (LDA or “pseudo fluid”, or “jellium” etc) [1, 2]. Special emphasis is made in present paper on the mentioned above non-ideality effects in non-uniform ionic subsystems, such as micro-ions profile within screening “cloud” around macro-ion in complex plasmas (dusty, colloid etc), in equilibrium ion distributions in ionic traps or in the neighborhood vicinity of “charged wall” etc. Multiphase EOS for simplified ionic model of classical charged hard spheres on uniformly compressible electrostatic compensating background (HS-OCP) was constructed in present work and several illustrative examples of discussed discontinuous ionic profiles in traps with different external potential were calculated with the use of this EOS in LDA approximation.

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Thermodynamics and transport properties of metals and rare gases in ionized fluid region

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Some thermodynamic and transport properties of gases with density of liquid and even a solid state in the presence of processes of thermal ionization are considered. Let us call for brevity such condition of substance an ionized fluid. One of the interesting effects found experimentally in recent years is the metallization of gases at compression. It is fixed in dense vapors of metals, at compression of inert and molecular gases. The unusual explanation of effect of metallization of metals vapors was offered in [1] with use of the “3+” chemical model. The conductivity increase at vapors compression was explained by existence of new component—electron jellium (sign “+” in the name of model in addition to traditional electrons, ions and atoms). Jellium arises from tails of the electron density of the ground state wave functions of all atoms lying out of atomic Wigner–Seitz cells. In the work with use of the “3+” model the comparative analysis of a role of jellium, intercharges and interatomic interactions in dense plasma of inert gases and vapors of metals is made. The small role of cohesive forces in dense rare gases with a significant contribution of jellium in conductivity is noted. The equation of state and electrical conductivity of alkali metals in near-critical region and for binodal are calculated within the “3+” model. Comparison with experimental results [2] is made. The offered simple model of the plasma fluid is rather successfully used in near-critical region of metals vapors and for dense plasma of rare gases. This work was supported by Presidium RAS program No. 13 “Condensed Matter and Plasma at High Energy Densities”.

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Problem of the third parameter of low-parametrical equations of state

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In the work, two groups of the equations of state (EOS) are analyzed. The EOS of van der Waals type is binomial cubic EOS with small (from 2 to 5) number of parameters included in the first group. Their main shortcoming—lack of communication with micro level. The second group includes the EOS, received on the basis of the prime molecular model—the interacting point centers (IPC). These are trinomial three-parametric EOS of two types depending on the nature of the interaction of point centers. These EOS have turned in two one-parameter families, the provision of the equation in which is defined by a value of one of two managing of parameters, the bound to a ratio of manifestation of attractive forces and a repulsion of point centers. In 145 years to the EOS of of van der Waals type the set of questions collected, main of which we call “a problem of the third parameter”. To what does conduct emergence in the EOS of the third parameter? Whether can be so that (as authors consider a van der Waals type EOS) two parameters would make former sense, and the sense of the new—is not defined? What its sense? Whether have the third parameters in different EOS the same sense? On these and other questions there are no answers at the standard approach to the EOS as to empirical modifications. If to exploit the opportunities of the IPCs model and to reformulate in it a van der Waals type EOS, then their main shortcoming is liquidated, connection with a molecular scale is established, the problem of the third parameter receives the decision and on many questions will be answered.

Free energy of defect formation in construction and fuel materials

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Atomistic simulation is an important tool for study the fundamental atomic processes such as diffusion of point defects. Diffusion of point defects in nuclear materials has an effect on many microscopic processes. The activation energy for defect diffusion is equal to the sum of the Gibbs free energies of defect formation and its migration. Since the free energy at non-zero temperature cannot be measured directly from molecular dynamics or Monte-Carlo simulations, its calculation must be performed using indirect methods. In this work we calculate Gibbs formation free energy of defects in bcc U and Mo following Frenkel and Ladd approach [1]. In this approach free energy difference between two states is calculated by thermodynamic integration over an ensemble average by coupling parameter λ . It allows us describe defect energetics at finite temperature and assess the quality of empirical interatomic potentials. The accuracy and limitations of the method are also discussed. The work is supported by the Scientific School grant No. 5922.2018.8 and by the Russian Foundation for Basic Research grant 18-08-01495.

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Accurate anharmonic theory and computation of defects in bcc metals

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Diffusion of point defects determines many microscopic processes in nuclear materials: climbing of dislocations, diffusion of fission products, formation of bubbles and swelling [1]. Experimentally measured self-diffusion is a combination of effects of vacancies and interstitials, and the contribution of interstitial atoms varies from insignificant to huge between different materials. The generally accepted model for temperature dependence of diffusion of defects is the Arrhenius equation $D = D_0 \exp[-E_a/k_B T]$, where E_a is a free energy barrier and D_0 is a frequency factor, determining an effective frequency of jump attempts [1]. However, bcc metals shows wide range of diffusion rate values comparing to fcc metals, and some of them like γ -U shows also deviation from linear law in Arrhenius coordinates [3]. Calculation of the diffusion coefficients and the equilibrium concentrations of point defects is important for building a mesoscale model of the evolution of a fuel in reactor conditions. In this work we use the molecular dynamics simulation to analyze the formation energies for Frenkel pairs in bcc U and Mo and its influence to the diffusion coefficient. The work is supported by the Scientific School grant No. 5922.2018.8 and by the Russian Foundation for Basic Research grant 18-08-01495.

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Density functional theory analysis of lattice vibrations in solid uranium

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Supercomputer modelling is a perspective way to study the processes, occurring in nuclear fuel. Mechanical properties of compounds of uranium are in many respects determined by the defect dynamics in crystal lattice. The defect mobility, in turn, depends on the vibrational properties of lattice, particularly on the phonon spectra and dispersion curves [1, 2]. The choice of the interatomic potential plays a key role in modelling. The results obtained by embedded atom model classical potential did not coincide experimental data enough [3]. Besides, more accurate results can be obtained using density functional theory (DFT) calculations [4], that demand much more computational time. To compare the accuracy and feasibility of using DFT calculations is an actual problem. In this work phonon density of states and dispersion curves for uranium were obtained with use of DFT calculations and compared with results of classical approach as well as the experimental data [5]. The impact of such calculation parameters like system size, number of k-points and cutoff energy on the result was analyzed.

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Mobility of edge dislocations in bcc uranium

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We perform molecular dynamics simulation of edge dislocation mobility in bcc uranium. Non-conservative (with increasing concentration of self-interstitial atoms) self-climb is observed. We have found this effect is increasing with temperature. Imposing external shear allows dislocation to glide and that makes climbing significantly greater.

How different methods are able to reproduce free energy

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The knowledge of free energy is crucial for determining phase stability of solids. In the present work we compare the accuracy of vibrational free energy calculation among different frequently used methods: self-consistent lattice dynamics, temperature-dependent effective potential, quasi-harmonic approximation, velocity autocorrelation function analysis and thermodynamic integration. Metals with two different types of lattices are considered as example: fcc Al and bcc Mo.

Ab-initio study of the phononic origin of negative thermal expansion

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Negative thermal expansion is an uncommon phenomenon of theoretical interest. Multiple hypotheses regarding its microscopic origins have been suggested. In this paper, the thermal expansion of a representative semiconductor, Si, and a representative metal, Ti, are calculated *ab-initio* using density-functional perturbation theory. The phonon modes contribution to the thermal expansion are analyzed and the negative thermal expansion is shown to be dominated by negative mode Grüneisen parameters at specific points on the Brillouin zone boundaries. Thus, the elastic (Debye) theory for negative thermal expansion is shown to be irrelevant for these phenomena. The anomalous behavior of these modes in Ti is shown to be unaffected by an electronic topological transition as previously suggested, instead it arises from complex interplay of atomic displacements of the anomalous mode [1].

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Atomistic study of the graphene nanobubbles

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A two-dimensional (2D) heterostructures can be created using 2D crystals stacking method. Substance can be trapped between the layers, which leads to formation of the surface nanobubbles. We study nanobubbles trapped between graphene layers with argon atoms inside using molecular dynamics approach. For bubbles with radius in range 7–34 nm the solid close-packed state of argon is found, although according to bulk argon phase diagram the fluid phase must be observed. The universal shape scaling (constant ratio of height to radius), which is found experimentally [1] and proved by the theory of elasticity of membranes, is also observed in our atomistic simulations. An unusual pancake shape (extremely small height to radius ratio) is found for smallest nanobubble with radius 7 nm. The nanobubbles with similar shape were experimentally observed at the interface between water and hydrophobic surface.

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Experimental study of liquid carbon

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A nanosecond-resolution pulse-heating technique was used to measure thermal expansion of pyrolytic graphite specimens. The change in the specimen volume was directly measured by means of a laser interferometer. The dependence of density of the graphite on specific enthalpy as well as the change in the specific volume upon melting has been measured at the pressures of 0.4–2 GPa. We have found that at the pressure of 1 GPa the specific volume increases upon melting by 30% from its solid state value of 0.52 cc/g, the heat of fusion is about 10 kJ/g and the electric resistivity of liquid carbon takes a value of 9 $\mu\Omega$ m. Also it has been found that for graphite at the pressures $P \leq 1$ GPa the isochoric temperature coefficient of resistance is positive, while for liquid carbon it is negative over the entire pressure range investigated. These observations probably indicate that graphite is a metal whereas liquid carbon is not a metal, so that the melting of graphite under such pressures coincides with a metal-to-nonmetal transition.

The supercooled diamond melt at near normal pressure

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We study at the first time of diamond melting at pressures close to normal rather than at megabar pressures typical of carbon exoplanets. The structural transformations of the diamond arise due to the contact with a drop of molten graphite with a pressure of 25 MPa. Using high resolution transmission electron microscopy, we define channels filled with cracked amorphous carbon. We establish the implantation of curved graphite monocrystals into diamond adjacent to a cracks at a depth smaller than 10 nm associated with the so-called explosive graphitization of diamond. Faceted nano-crystals of graphite are embedded into diamond and into a crack at a depth cca 50 nm. Only liquid carbon may be occupied a twice volume over diamond [1], and thus the second structure we connect with the solidification of the diamond melt. Surprisingly, that reaction on diamond volume superheating is only the defects growing, but quick fragmentation of the same diamond provides its melting solution. In view of relationship between the critical nucleus diameter and the supercooling below melting temperature nano-graphite is indicative that the molten diamond was in a highly supercooled state. Really the melting temperatures differs essentially for the metastable at chosen pressure diamond (4160 K [2]) and stable graphite (4850 K [3]). The work was funded under the Russian Academy of Sciences Program N13.

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Dependence of structure of amorphous carbon upon the speed of quenching of liquid carbon: Classical molecular dynamics simulation

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We describe the effect of the cooling rate on some structural properties of amorphous carbon obtained using classical molecular dynamics simulations. Quenching has been carried out using a linear velocity rescaling. In the present paper we discuss the influence of the initial liquid configuration on the structure of amorphous carbon. Structural properties of both liquid and amorphous samples are compared. Our results confirm that in classical molecular dynamics simulations as in experiment, quenching is the crucial step for structural changes between the liquid and amorphous phase.

For molecular dynamics simulation we used LAMMPS—Large-Scale Atomic (Molecular) Massively Parallel Simulator software package. The initial simulation cell is a cube with an edge of 57 Å and periodic boundary conditions, containing 11408 carbon atoms. Interaction between the carbon atoms (in liquid and in amorphous states) was determined by a classical bond-order potential ReaxFF. To investigate the influence of the quenching rate on the structure of amorphous carbon we study bulk quenching from liquid carbon in the *NPT* ensemble at constant pressure about 1 GPa. Above all, we are interested in how the distribution of chemical bonds, sp^1 – sp^2 – sp^3 in amorphous carbon depends on the quenching rate of liquid carbon.

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High temperature nucleation of carbon vapor at different densities

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The applicability of such carbon nanostructures as graphenes, fullerenes, nanotubes in industrial areas (energy, electronics, aviation, etc) is great due to the interesting properties of materials (increased strength, resistance, heat and electrical conductivity, etc). It is known that such parameters of synthesis as temperature, pressure and gas density in the most critical manner affect on the formation of the structures and on its geometry. The aim of this paper is to investigate the parameters that will help to simplify and to understand the mechanism of nucleation of carbon structures. To identify the highest yield of the carbon nanostructures it is necessary to assess the degree of influence of the gas density on clusterization. After comprehensive study and determination of the most advantageous parameters, it will be possible to obtain these compounds on an industrial scale. The accuracy of modern quantum mechanical and quantum chemical methods make it possible to predict some properties of small molecules accurately. However, calculations using quantum methods are not yet suitable for studying large molecules and solids because of the high computer costs. As a consequence, a detailed theoretical study of the nucleation of carbon structures is carried out using molecular dynamics methods using reactive interatomic potentials (ReaxFF and AIREBO). They have quantum accuracy due to quantum-mechanical parametrization and spend less computer time.

Equations of state for pentaerythritol tetranitrate and its explosion products based on atomistic simulation data

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Equation of state (EOS) and transport coefficients are of importance for hydrodynamics modeling of explosives. The conditions typical for the initiation and propagation of detonation are characterized by high pressure and high temperature both for reactants and products. The rates of the chemical reactions are very high as well. That all makes it impossible to directly measure thermodynamic parameters during those processes. Atomistic simulation allows to calculate the parameters in a wide range of conditions. This work presents the equations of state for pentaerythritol tetranitrate (PETN) and its explosion products based on the molecular dynamics (MD) and quantum mechanical data. To determine the high-temperature part of EOS we carried out a set of MD simulations with the ReaxFF-*lg* interatomic potential at different densities and temperatures in the LAMMPS code. The results are in good agreement with quantum mechanical calculations and experimental data. For every state we calculate pressure and internal energy, that allows us to obtain the EOS in the Mie–Grüneisen form. We show that at temperatures below 2000 K for PETN and 1000 K for its explosion products the heat capacity can not be described from the classical point of view. The heat capacity in this range is obtained with the quantum-mechanically calculated phonon density of states (PDOS). The PDOS is obtained with the finite displacements method using the VASP and Phonopy codes. Above the indicated temperatures the values of heat capacities approach the classical limit.

The tensors of thermal expansion of molecular crystals pentaerythritol tetranitrate and hexanitrobenzene

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The tensors of thermal expansion for pentaerythritol tetranitrate (PETN) and hexanitrobenzene (BTF) are calculated from powder x-ray diffraction data in the temperature range from 150 to 380 K for PETN and from 150 to 470 K for BTF. The points of structural changes of energetic materials was by increments of 10 K. Calculations of x-ray diffraction data were performed using full-profile analysis integrated into the algorithm by loop quantum modeling of molecular structures [1]. As reference methods used a full-profile analysis method Pawley [2], Le Bail [3], Rietveld [4] (WPPD) and WPPM [5]. The main crystallographic axis and the characteristic surface of the tensor of thermal expansion were determined. The tensor of thermal expansion and the temperature dependence are presented numerically, algebraically and graphically. The obtained results can be used to construct equations of state of condensed BTF and PETN.

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The equilibrium morphology and faceting of high-explosive molecular crystals

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Theoretical and experimental methods were used to analyze the equilibrium morphology of high-explosive (HE) crystals formed in the framework of technological models of ideal mixing and ideal displacement. The equilibrium faceting of HE crystals, the relative surface of the crystal faces, the habitus and the texture are calculated using the Bravais–Friedel–Donnay–Harker [1, 2], attachment energy [3], equilibrium morphology [4] and growth morphology [5, 6] methods. The correspondence between the morphology of the HE crystals and the theoretical calculations has been established by optical and electron microscopy. On the example of HE molecular crystals, it is proved that in the process of formation of crystalline materials, the violation of models of ideal mixing and ideal displacement in a chemical reactor lead to the formation of various forms of defects: dislocations, twins, pores and others.

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Temperature distribution and emissivity under high pressure and high temperature

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Diamond anvil cell (DAC) is the only experimental tool to study the properties of materials under high pressure and temperature under static conditions. It is widely used in high pressure research and geophysics. In this report, we describe further development of a multi-functional in-situ measurement system under high pressure and temperature equipped with imaging tandem acoustic-optical tunable filter (iTAOTF), Raman spectrometer, laser ultrasonic (LU) and laser heating (LH) system in a DAC. Spectroscopic devices allow to measure integral temperature of the objects by using Planck's law. Recently it was shown that iTAOTF synchronized with a video camera allows in-situ measurement of the temperature distribution and emissivity over the surface of microscopic specimens. Both methods of measurement (an integral temperature and 2D distribution of the temperature) can be realized in our system. The comparison of the data shows good correlation of the results. The usage of iTAOTF gives further advantages. The laser heating requires knowledge of the precise focus position of IR laser beam. iTAOTF provides a method to visualize the IR laser beam, invisible to human eye, that is widely used for laser heating in DAC. Also iTAOTF makes it possible to control the distribution of the laser incident on the sample during the experiment. It will allow us to heat more precisely and to apply numerical method describing the heat propagation in a media for the determination of the thermal parameters of solids and liquids under high pressure and temperature.

Development of laser heating system for study of material properties under high pressure and temperature

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We report on the development of the laser heating system for high temperature and high pressure studies with precise in-situ control of these parameters. One of the main features of the system is an imaging acousto-optical tunable filter. It provides measurements of the temperature distribution over the surface of the microscopic samples. High-resolution diffraction spectrometer is used for the measurements of reflectance, fluorescence and Raman scattering necessary for pressure control and one-point verification of the results obtained by acousto-optical tunable filter. We conducted multiple temperature measurements using both techniques and confirmed their effectiveness. It was found that temperature of tungsten lamp heated by constant current from a stabilized current source measured by acousto-optical tunable filter is in excellent agreement with that measured by diffraction spectrometer. We also demonstrate that the proposed system may be used for in-situ high temperature distribution and high pressure measurements in the iron samples.

Novel algorithm of hyperspectral imaging data processing for temperature distribution determination on laser heated materials in high pressure cells

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Laser heating is one of the main tools in the study of minerals and synthesis of new materials under high pressure and temperature in a diamond anvil cell. It is a challenge to measure the two-dimensional temperature distribution inside a spot heated by a laser beam in a diamond anvil cell. It is demonstrated that combining a laser heating system with an acousto-optical filter allows determination of the temperature distribution in a diamond anvil cell during the laser heating. We develop an algorithm for fast data treatment of the hyperspectral imaged obtained by the acousto-optical imaging filter. This algorithm determinates the temperature distribution in a graphitic specimen heated by ir laser in pressures range up to 25 GPa. The maximal temperature at the peak was ≈ 4000 K. Spectra data were collected by a novel acousto-optical spectrometer operating in the spectral range 630–1100 nm. It is shown, that the algorithm is an effective tool for hyperspectral imaging data processing to the determination of the temperature distribution in materials under high pressures in a diamond anvil cell. Research funded by Russian Science Foundation grant No. 17-12-01535.

Reaction of fayalite with hydrogen at high pressure

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Fayalite is the end-member compound of olivine—the most abundant mineral in the upper Earth mantle. Studies on the pressure-induced phase transformations in olivine play a key role in understanding the processes occurring in this part of the Earth interior. Investigating the interaction of olivine with gases at high pressure is of no less importance because the Earth crust and upper mantle contain lots of various gases, too. As the starting material, we used the fayalite powder synthesized by solid-state reaction of silica, carbonyl iron and hematite at $T = 1000$ °C in the reduced atmosphere. Powder samples were then exposed to an H₂ atmosphere at $P = 7.5$ GPa and $T = 280$ °C for 24 hours, quenched to -196 °C to prevent hydrogen losses after the pressure release and further studied in the quenched state at ambient pressure and $T = 85$ K by x-ray diffraction and Raman spectroscopy. According to these studies, the hydrogenated samples of fayalite completely decomposed to a mixture of iron hydride with a double-hcp crystal structure and coesite, a high-pressure phase of silica. The work was supported by the Program “Elementary Particle Physics, Fundamental Nuclear Physics and Nuclear Technologies” of the Russian Academy of Sciences.

Thermoelectric properties of $\text{Fe}_{2-x}\text{V}_{1+x}\text{Al}$ half-Heusler compounds at high pressure up to 10 GPa

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Fe_2VAl is one such class of alloys that has been the topic of interest over the past decade because of its rich variety of unusual transport and magnetic properties. Recent works confirm existence of a sharply varying electron density of states and a strong scattering of charge carriers by magnetic inhomogeneities in Fe–V–Al alloys with a composition variation near the stoichiometric one [1]. In the present work the behavior of thermoelectric (TE) power and electrical conductivity of $\text{Fe}_{2-x}\text{V}_{1+x}\text{Al}$ (where $-0.1 \leq x \leq 0.2$) half-Heusler compounds was investigated under high pressure application up to 10 GPa at room temperature using an automated set-up (mini-press) operating miniature anvil-type high-pressure cell with anvils made of hard-alloys [2]. It was found that application of moderate pressure up to 1–2 GPa caused two-fold increasing of TE power factor value for $\text{Fe}_{2.1}\text{V}_{0.9}\text{Al}$ compound.

The work was supported by the Federal Agency for Scientific Organizations Russia (subject “Electron” No.01201463326) and the Russian Foundation for Basic Research (grant No.18-32-00618).

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Electrical properties of new oxide ceramics $\text{Sr}_2\text{Mn}_{0.5}\text{Ti}_{0.5}\text{O}_4$

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A new complex oxide $\text{Sr}_2\text{Mn}_{0.5}\text{Ti}_{0.5}\text{O}_4$ with K_2NiF_4 -type structure was produced under thermobaric conditions. The structure, microstructure and electrical properties in a wide range of temperatures and pressures have been studied. It was found that ceramics possess a giant dielectric constant and exhibits a negative magnetoresistance at pressures above 16 GPa. The mechanism of negative magnetoresistance is being studied. This work was supported by the Russian Foundation for Basic Research (grant No. 16-02-00857) and acknowledged by the financial support of Federal Agency for Scientific Organizations of Russia Institute of Solid State Chemistry of the Ural Branch of the Russian Academy of Sciences.

The influence of dc on the morphology of the surface of bulk amorphous composites

$\text{AgGe}_{1+x}\text{As}_{1-x}(\text{S}+\text{CNT})_3$, $x = 0.5, 0.6$

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In this work the change in the surface morphology of amorphous silver chalcogenides $\text{AgGe}_{1+x}\text{As}_{1-x}(\text{S}+\text{CNT})_3$, $x = 0.5$ and 0.6 under the influence of a constant external electric field were investigated. The sample was fixed between two graphite electrodes and a constant voltage was applied to the cell. Under the influence of an external field conductive filaments from silver ions are formed inside these materials. At the first moment when the dc voltage is applied to the sample, the ion current is directed towards the negative electrode. With according to the cathode deposition reaction on the surface of the sample adjacent to the negative electrode, a neutral silver layer is deposited. Silver forms fractal structures on the surface of $\text{AgGe}_{1+x}\text{As}_{1-x}(\text{S}+\text{CNT})_3$, $x = 0.5$ and 0.6 . At the same time, on the surface of the material near the positive electrode defects in the form of craters and depressions are appeared, which may be due to the following processes. At the moment when the dc voltage is turned on, the silver ions form the conductive filaments and move toward the negatively charged electrode and consequently voids arise in the places where silver ions were located previously, that leads to the mechanical softening of glass. It should be noted that the process of formation of fractal structures from silver on the surface of $\text{AgGe}_{1+x}\text{As}_{1-x}(\text{S}+\text{CNT})_3$, $x = 0.5$ and 0.6 is reversible. When applying a constant voltage with reverse polarity, these structures can be completely dissolved in accordance with the anodic dissolution reaction. The study was supported by the Russian Foundation for Basic Research (grants 16-02-01137, 16-02-00857).

Negative magnetoresistance of the polycrystalline materials from the system Cu–As–Ge–Se under high pressure

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This work is devoted to the phenomenon of negative magnetoresistance (NMR) under high pressure (P) (up to 50 GPa) in the polycrystalline material $(\text{GeSe})_{1-x}(\text{CuAsSe}_2)_x$, $x = 0.3, 0.5, 0.6$. The semiconductors materials $(\text{GeSe})_{1-x}(\text{CuAsSe}_2)_x$ are promising objects for investigating because of its interesting thermal and electrical properties [1, 2]. To measure magnetoresistance under pressure up to 50 GPa in transverse magnetic field (up to $B = 1$ T) high pressures have been generated in the cell with synthetic carbonado-type diamond anvils [3]. It was found that all studied materials manifest NMR (up to $\approx 60\%$ in modulus) under high pressure. There are several extremes on curves $\text{NMR}(P)$ for materials $(\text{GeSe})_{1-x}(\text{CuAsSe}_2)_x$, $x = 0.3, 0.5, 0.6$ as well as for materials $(\text{GeS})_{1-x}(\text{CuAsS}_2)_x$ [4]. This extremes correspond to the pressure intervals of the other electrical properties behavior features (electroresistance, tangent of dielectric loss, thermo-EMF). The material $(\text{GeS})_{1-x}(\text{CuAsS}_2)_x$, $x = 0.3$ can be obtained from material $(\text{GeSe})_{1-x}(\text{CuAsSe}_2)_x$, $x = 0.3$ by isovalent replacement of selenium atoms to sulfur atoms. Such replacement leads shift of $\text{NMR}(P)$ extrema [5]. The study was supported by the Russian Foundation for Basic Research, projects No. 16-02-00857.

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The effect of thermobaric treatment and isovalent substitution on high values of the permittivity $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$

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At present known the perovskite-like materials $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ have a high value of the permittivity ε (10^3 – 10^4) [1]. These materials attract the attention researchers concerned that there is, reasons for high value of ε not yet been studied in detail. For the purpose of studying, how powerful can be to change polarization density on ε $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$, was conducted isovalent substitution of a parts of Ti atoms by V and Zr atoms. Samples synthesized by solid-phase synthesis with subsequent thermobaric treatment. The conditions and the equipment of the synthesis are described in [2]. Possible causes for a high value of the permittivity are reviewed, such as: effects at sample-electrode interface (Schottky barriers), Maxwell-Wagner polarization or Internal Barrier Layer Capacitors (IBLC-model) these are internal causes, polarization density and nanoscale effects-Nanosized Barrier Layer Capacitance (NBLC) and polaronic relaxation these are external causes. Experimental results better described by NBLC model and hopping mechanism of small-polaron conductivity [3]. This work was supported in part by the Russian Foundation for Basic Research, projects No. 16-02-00857.

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Three-dimensional granular dynamics simulations of polydisperse and bidisperse nanopowders compaction processes

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Processes of nanopowders uniform compaction have been simulated in 3D-geometry. Parameters of interaction laws correspond to the oxide powders with strong tendency to the agglomeration, i.e., the systems of II type in [1, 2]. The study continues [3], where the similar investigation was performed in 2D-geometry. As a result of the present study, polydisperse systems with the log-normal particle size distribution of different width as well as bidisperse systems with the different content of small particles (with diameter of 10 nm) and large ones (30 nm) have been investigated. It is revealed for the polydisperse systems that the increase of the distribution width from zero up to the value, which corresponds to real nanopowders, has an insignificant influence on the compact density. The nonmonotonic dependence of density on the weight fraction ω_m of small particles has been revealed in the bidisperse systems; namely, the dependence $\rho(\omega_m)$ has a maximum in the vicinity of $\omega_m = 0.35$, where the bidisperse system density can exceed by 6% the densities of corresponding monosystems. The study has been performed within state programme 0389-2014-0002 and partially supported by the Russian Foundation for Basic Research (project 16-08-00277).

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Experimental investigation of the phase formation in the NaF–CePO₄ system

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One of the promising technologies for processing monazite, which is the main rare-earth mineral raw material, is liquation melting [1], carried out in the presence of the third component, which is NaF. The content of rare-earth elements in monazite varies from 45 to 60% and the main quantity (up to 90%) falls on the share of lanthanum and cerium. Studies of NaF–phosphate lanthanide systems are aimed at modeling the behavior of lanthanides in the process of liquation melting and determining the amount of rare earth phosphates that can be dissolved in the melt of sodium fluoride. In [2] such studies were performed for the NaF–LaPO₄ system. In this paper the results of the investigation of the system NaF–CePO₄ are presented. The experiments were carried out with the help of the thermal analyzer SDT Q600, which allowed to use simultaneously thermogravimetric analysis and differential scanning calorimetry. As a result of the studies, it was shown that the NaF–CePO₄ system is a eutectic-type system. Its phase diagram was constructed, the temperature of formation and the heat of melting of the eutectic were determined, as well as the mass content of NaF and CePO₄ in its composition. The behavior of lanthanum and cerium phosphates was compared. The work was supported by the Russian Foundation for Basic Research, grant No. 17-08-00583.

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Investigation of evaporation behavior of ZrC_x at temperatures above 4000 K

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Zirconium carbide is a promising material for different applications at high temperatures, for example, thermal protection. Such applications demand knowledge on the behavior of the material at high temperatures. Previous high-temperature studies of the material were performed using stationary heating techniques [1–3]. In [4] congruently evaporating composition of zirconium carbide was found in solid state. Although methods used allow to obtain reliable thermodynamic data they has temperature limit at 3200 K. In present work, laser heating was applied to study the evaporation behavior of zirconium carbide over wide range of temperatures (3400–4300 K). For the first time the evaporation of liquid ZrC_x with various initial compositions ($x = 0.68\text{--}1$) was studied. Time-of-flight mass-spectrometry with millisecond laser pulses were applied to find the temperature dependence of vapor composition. Partial pressures of $\text{C}_1\text{--C}_3$, zirconium isotopes, ZrC , ZrC_2 and Zr_2C were obtained. With increasing of the temperature the C/Zr ratio was shown to decrease over the ZrC_x with $x > 0.9$ and slightly increase for $x < 0.9$. It was found that the C/Zr ratio over the samples with different initial compositions tends to the value of about 0.2 above 4000 K.

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Measurement of the emissivity of metals under extreme conditions

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The laser-heated diamond-anvil cell (LH-DAC) is currently the only experimental tool able to create extreme static pressures (up to 300 GPa) and temperatures (up to 6000 K) [1] and is therefore widely used in studies of phase transitions and for the synthesis of new superhard materials. This method provides obtaining such pressures and temperatures that occur in the bowels of the Earth and are often used for mineralogical research. Further progress in high-pressure physics and in the physics of minerals is closely related to the development of these methods, in particular to the development of methods and means for measuring the distribution of emissivity in high-pressure cells under laser heating. In this study, we propose a new method for measuring the distribution of the emissivity [2] of samples, based on the spectral imaging of a heated sample at several wavelengths in a sufficiently wide spectral interval, determining the spectra at all points, and calculating the emissivity in them. The uniqueness of this method is the ability to obtain a visual representation of the spatial distribution of the radiation coefficient in the region of sample heating [3].

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Determination of the true temperature of an opaque material in a condensed state from the spectral distribution of radiation temperatures

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As is known, determination of the thermodynamic (true) temperature of an opaque free-radiating material in a diathermic medium has several advantages over contact methods. First of all, this is recording the thermal radiation of the material without direct contact with the object of measurement, as well as high speed. These properties are especially important in determining the temperature in fast processes. For example, under the influence of high-energy flows on matter. In addition, it is possible to register radiation fields using only one measuring instrument by changing the direction of the sight. The report presents graph-analytical methods for estimating the thermodynamic temperature of opaque materials in a condensed state. As an example, a tungsten sample heated to a temperature above 1200 K is considered.

Investigation of thermal expansion of refractory metal carbides at high temperatures with pulse heating technique

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The experimental study of the thermal expansion of refractory carbides (e.g., TaC, ReC, TiC, WC), and in particular the effect of stoichiometry of carbides on the thermal expansion coefficient (CTE) under fast electric heating 10^5 – 10^7 K/s are of great interest nowadays. The dependence of the CTE of refractory carbides on their stoichiometry is an important factor for their practical use and theoretical study.

The novelty of the proposed approach is the use of precision technology of optical pyrometry, high-speed digital visualization of the thermal expansion of the materials under study, as well as the possibility of using various heating rates. The chosen approach allows us to investigate the CTE of refractory carbides over a wide range of high temperatures for stoichiometries previously unstudied.

Direct measurement of the sample temperature makes it possible to switch off the heating at a given temperature in real time (during the experiment). This allows us to investigate the change in the microstructure of the sample (after the experiment) after it reaches a predetermined temperature, which provides a study of the phase behavior of the sample upon heating and control of the change in its stoichiometry, which is especially important for refractory carbides.

Method of investigations of thermal conductivity of metals in the field of centrifugal accelerations

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In the work, the method of investigations of thermal conductivity of materials in the field of centrifugal radial and district accelerations has been developed. A device with a heat conductors to determine thermophysical characteristics of materials on the spin rig using the vacuum chamber in conditions of centrifugal radial and district accelerations has been developed. From the analysis of the results of experimental investigations it may be stated that the thermal conductivity (heat transfer time) of the heat-conductors increases significantly with an increase of a rotation frequency compared to the steady state. Thus, this increase of the thermal conductivity significantly associated with an increase of the electron drift velocity under the influence of centrifugal accelerations. The obtained results are of practical importance for the assessment of the thermal state of the rotating parts of aircraft engines and other energy turbomachines.

Transport properties of topological insulators

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Transport properties of topological insulators [1] are calculated within Bastin–Kubo–Streda formalism. We take into the account particle-hole asymmetry and hexagonal warping of the surface states [2]. We found that increase of the disorder unexpectedly leads to increase of the longitudinal conductivity for large disorder. Anomalous anisotropic magnetoresistance is incommensurate with the crystal symmetry. Hexagonal warping is responsible for additional components in the spin conductivity tensor. Good comparison with available experiments on bismuth selenide and bismuth telluride compounds is found [3].

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Transport properties of proton-exchange membranes with a short side chain

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Proton-conducting membranes were obtained by the solution casting method from new ionomer Inion (Russian analog of Aquivion). For this purpose, a small amount of ionomer solution, was uniformly casted on a glass substrate. The amount of the ionomer solution was selected experimentally; as a result, 0.8 ml of 3 wt % solution was enough to form a thin film and optimal for uniform evaporation of the solvent throughout the entire thickness of the membrane without its cracking. To increase the thickness of the membrane, the same amount of solution was casted on the surface of the previous layer, dried at standard conditions for one hour. Thus, three layers of the solution formed a membrane with a thickness of approximately 20–30 m. Finally, the thermal treatment of membranes was carried out: samples were annealed for 20 h at fixed temperatures in the range from 80 to 220 °C. It is shown, that annealing of membranes at temperature range from 160 to 170 °C leads to significant increase of specific proton conductivity to values even higher, than those of commercial membrane Nafion NR212. In this case, these membranes are of undoubted interest as they can be practically used in effective hydrogen–air fuel cells. One of the authors (Mugtasimova K. R.) thanks the “UMNIK” foundation (9882/2015) for her financial support.

Elastic properties of 1-propanol at high pressure

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1-propanol is a monohydric alcohol with 1 hydroxyl group OH, which can organize a hydrogen bond with two neighboring molecules. Previously, we have studied the influence of hydrogen bonds on the elastic properties of dihydric and trihydric alcohols (propylene glycol and glycerol) [1]. The ultrasonic investigation of 1-propanol allows to qualitatively compare the dependence of the elastic properties of alcohols on the basis of the propane carbon skeleton on the number of hydrogen bonds per molecule. 1-propanol has high baric derivatives of ultrasound velocities at room temperature, as well as an anomalous compressibility in the liquid phase [2]. Thus, we have seen a decrease in the volume of propanol at room temperature by 30 percent at pressures up to 1 GPa. The elastic properties of 1-propanol were studied in the liquid state (room temperature 295 K), in the glassy state (77 K), and also at the heating (77–295 K) during the glass–liquid transition. The compressibility of glass is much less than that of liquid, and the ultrasound velocity is more than 2 times higher in the glassy phase (the longitudinal ultrasonic wave velocity is 1.2 km/s at 295 K and 2.6 km/s at 77 K). There is a sharp drop of the ultrasound velocities and the elastic moduli during devitrification. The shear modulus G disappears upon transition to a non viscous liquid state, and the bulk modulus B decreases from 4.5 GPa (77 K, glass) to 1.5 GPa (295 K, liquid).

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Lattice twinning and detwinning relations and variant formation in shape memory alloys

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Shape memory effect is based on successive martensitic transformations; thermal induced and stress induced martensitic transformations. Martensitic transformation is first order lattice-distorting phase transformations, and occurs with cooperative movements of atoms by means of shear-like mechanism. Shape memory alloys recover the original shape on heating over the austenite finish temperature after deformation at low temperature martensitic condition. Martensitic transition occurs as martensite variants in self-accommodated manner with lattice invariant shears on the $\{110\}$ -type close packed planes of austenite matrix. The $\{110\}$ -plane family has 6 specific planes; (110) , $(\bar{1}10)$, (101) , $(\bar{1}01)$, (011) and $(01\bar{1})$. Lattice invariant shears occur in both sides of these planes; therefore crystallographically equal 24 martensite variants occur in different orientations Thermal induced martensite occurs as twinned martensite, and the twinned structures turn into the detwinned structures by means of strain induced martensitic transformation by stressing the material in the martensitic condition. Deformation of shape memory alloys in martensitic state proceeds through a martensite variant reorientation. Copper based alloys exhibit this property in metastable β -phase region, which has bcc-based structures at high temperature parent phase field. Lattice invariant shear and twinning is not uniform in copper base shape memory alloys and causes to formation of the long period layered structures. In the present contribution, x-ray diffraction and transmission electron microscopy studies were carried out on two copper based ternary alloys. The x-ray diffractograms taken in a long term interval reveals that diffraction angles and peak intensities change. This result leads to the rearrangement of atoms in diffusive manner.

Effect of stoichiometric composition on physical-mechanical properties of CoCrFeMnNi high-entropy alloy

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Structural and physical-mechanical properties of CoCrFeMnNi high-entropy alloys (HEAs) of different stoichiometric compositions were investigated. To describe the interatomic interaction in CoCrFeMnNi, manybody potentials [1, 2] constructed within the framework of the second nearest neighbor modified embedded atom method were used. These potentials describe the lattice parameters, elastic moduli, structural features and energy parameters of extended defects with a high degree of accuracy, as well as the thermodynamic behavior of various phases of the material, etc, which is important for the correct simulation of HEAs. An approach based on the combined use of molecular dynamics and Monte Carlo methods was applied. It allowed to obtain the thermodynamically equilibrium configurations of CoCrFeMnNi alloys at given concentrations of chemical elements, temperature and pressure. Based on the obtained data set, the influence of the stoichiometric composition of the CoCrFeMnNi HEA on its structural characteristics (lattice parameter, radial distribution functions), phase stability (energy of different phases, configurational entropy) and physical-mechanical properties (elastic moduli, stacking fault energy, elastic limit, melting point, diffusion coefficients) was investigated. The work was carried out with the financial support of Russian Science Foundation (project No. 17-79-10108).

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Galvanomagnetic properties in Fe–V–Al alloys in the vicinity of stoichiometry

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The main task of our investigations is to reveal the specificity of the electronic structure of iron–vanadium–aluminum alloys (Fe_2VAl), with a variation in composition near the stoichiometric one. One of the results concerning alloys it is a strong effect of aluminum content on the magnitude and character of the development of spontaneous magnetization. To study and analysis of the magnetoresistance and anomalous Hall effect of Fe–V–Al alloys with a composition change near the stoichiometric, both for iron atoms and for aluminum atoms, is performed in this paper. From the temperature dependence of the resistivity, we observed characteristic maxima, which indicate the presence of a ferromagnetic phase transition [1,2], from which it was concluded that even a slight deviation from stoichiometry in the direction of increasing Al content leads to a significant increase in the Curie temperature. An investigation of the Hall effect showed that the additional alloying of the alloy with Al atoms leads to a change in the sign of the anomalous contribution from the negative (Al-enriched sample) to the positive (the sample enriched with Fe and Al) above 10 K. The obtained data confirm the existence of a sharply varying electron density of states and a strong scattering of charge carriers by magnetic inhomogeneities in alloys with a composition variation near the stoichiometric one. The work was supported by the Federal Agency for Scientific Organizations of Russia (subject “Electron” No. 01201463326) and the Russian Foundation for Basic Research (grant No. 18-32-00618).

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Adsorption relaxation of a freshly formed metal surface in a vacuum

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Using equation

$$\sigma = \sigma_0 + RT\Gamma\left(\frac{S_0bp}{1 + S_0bp}\right)\left(1 - \exp\frac{-t}{\tau_P}\right),$$

that proposed by the authors of the present communication, it is possible to describe the kinetics of interaction freshly formed surface of the metal with the residual gas of the vacuum system research camera. It is shown that one of the reasons noted in the literature, the dispersion of the values of surface tension of pure metals is the adsorption of residual gas molecules on the surface of the liquid metal.

Efficiency of superhydrophobic coatings for mixing of shear thinning fluid in microchannel

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The efficiency of the superhydrophobic striped texture for mixing of a shear thinning polymeric fluid in a microchannel was studied by means of numerical simulation. The mixing intensity was suggested to describe in terms of the average tangent deflection angle of the streamlines through the volume of the microchannel. Dependence of this characteristic on the inclination angle of the striped texture to the main flow direction was investigated at different flow velocities for Newtonian and shear thinning fluids. It was found that the use of the anisotropic superhydrophobic coating for mixing of the shear thinning fluids is less efficient than for Newtonian ones. The mixing intensity of the shear thinning fluids was found to be strongly dependent on the average flow velocity while the optimal inclination angles of the superhydrophobic striped texture are different from that of Newtonian liquids.

Flow bifurcations of shear thinning fluid in two-dimensional channel with sharp contraction and expansion

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In this work, numerical modeling of the pressure driven flow of the shear thinning fluid in a two-dimensional channel with the variable cross-section was carried out. As a shear thinning fluid, the aqueous solution of polyacrylamide, whose viscosity decreases with increase in shear rate, was considered. The flow stability of such a medium was investigated within the framework of the Carreau–Yasuda model at different Reynolds numbers. It was found that bifurcation of the symmetric vortex flow of the non-Newtonian fluid to an asymmetric state occurs at lower Reynolds numbers than for similar Newtonian fluid with a viscosity equal to the zero shear rate viscosity of the shear thinning fluid. This kind of behavior was explained due to a sharp drop of viscosity near the narrowing part of the channel.

Deformation behavior of highly viscous droplet upon inflowing into narrow slit

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The numerical modeling of the hydrodynamic behavior of the highly viscous 3D droplet upon inflowing into to a narrow slit of a flat microchannel at low Reynolds numbers has been carried out. The attention focused to the investigation of peculiarities of the droplet deformation behavior as a function of the confinement parameter as a ratio of the unperturbed droplet diameter to the gap thickness. It was found that droplet entering into the narrow slit from the wide part of the channel was subjected to the sudden stretching due to a large velocity gradient along the channel axis. The further motion of the droplet through the slit resulted in its slight relaxation induced by the capillary forces. The degree of droplet elongation was found to be sensitive to values of the confinement parameter and Reynolds number.

The effect of spin polarization on recombination dynamic of dislocation induced defects in Si

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Recently, on previous conference, we have reported about generation of new types paramagnetic defects in Si as a result of plastic deformation of samples enriched with ^{29}Si . Later on it was shown that dislocation related lines in Si D1 and D2 are sensitive to the presence and orientation of external magnetic field. Effect of influence of spin polarization on the recombination dynamic is rather important from point of view of application this material in cubit technology. The presence of this effect in Si is especially important, because Si is the mainstream semiconductor. The existing technology base for Si makes it more favorable to investigate the spin-related phenomena. The paper presents the new experimental data of investigation the effect in plastically deformed ^{29}Si .

Resonant collective dynamics of the weakly pinned soliton lattice in a monoaxial chiral helimagnet

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We study the spin dynamics of a confined chiral soliton lattice whose ends are weakly held. We demonstrate that in this case the system possesses its own resonant frequency. To study features of the resonant dynamics, we analyze the collective motion of the system driven by an oscillating magnetic field directed along the chiral axis. By using the method of collective coordinates we find analytically the resonant frequency and verify the result by numerical simulation of the spin dynamics with the aid of Landau–Lifshitz–Gilbert equations. The numerical simulation shows an appearance of the asymmetric profile of the frequency response function with increasing ac field, which is typical for a nonlinear resonance. To give an explanation of this behavior, we invoke the multiple-time-scale method and predict an emergence of hysteresis phenomena. We also demonstrate that the spin-motive force is strongly amplified by the resonant oscillations.

Thermodynamic properties of the argon hydrides ArH^+ and ArH

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The charged diatomic compounds are important for different plasma sources, that contain argon as basic gas. One of such essential application is mass spectrometry with inductively coupled plasma (ICP-MS). For accurate prediction of the final measurement results is necessary to have data about thermodynamic functions of the diatomic argon compounds. However, thermodynamic properties of the dimeric ion of argon are not sufficiently studied. Recently we performed accurate calculations of the internal partition functions for various diatomic argon compounds (VAr^+ , CoAr^+ [1] and Ar_2 , Ar_2^+). In this work we report the calculation of the internal partition functions of the ArH^+ and its precursor ArH . The data of the potential energy function in the ground state of the ArH^+ was taken from [2] and for excited states from [3]. For neutral molecule were taken into account ground state from [4] and also excited states from [5]. Using received data the one-dimensional Schrödinger equations was solved using the Level code (v. 8.2) [6] and the internal partition functions were calculated with developed Partition function code. Calculations of the thermodynamic functions of ArH^+ and ArH have been performed using procedures set out in the reference book [7].

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Atomistic modeling methane–n-pentane evaporation curve

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In this work, we study the vapor–liquid equilibrium in methane–n-pentane. We use the TraPPE–EH (transferable potentials for phase equilibria–explicit hydrogen) forcefield, where each hydrogen and carbon atom is considered as independent center of force.

The use of capillary oscillations and atomic force microscopy to determine the surface and linear tensions of microdroplets of metallic melts

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Capillary properties of microparticles can not be correctly described without taking into account the linear tension arising on the line of the interphase contact [1, 2]. The magnitude of the linear tension can be determined from the dimensional dependence of the contact angle between droplet under investigation and solid substrate [2]. Despite the importance of this topic, there is no reliable data on linear tension in the metal microdrop—solid substrate system in the literature. In this study, an attempt has been made to apply capillary oscillations [3] and elements of atomic force microscopy [4] to determine the contact angle of wetting, surface and linear tension in a low-melting metal–silicon oxide system. Measurements are taken from the image of microdroplets of gallium and its alloys, obtained by their illumination with fast electrons.

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Fluctuation enhancement of ion diffusivity in liquids

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Diffusivity of ions in liquid solutions determine ionic mobility and conductivity of a liquid, rate of diffusion-controlled reactions. The majority of models of the diffusion in dilute liquid solution predicts monotonic decrease of the ion diffusivity with ion size or a maximum in the dependence of ion diffusivity on ion size. It is shown that there may be multiple maxima in the dependence of ion diffusivity on ion size. Ion motion could be separated into a motion together with solvation shell as a whole and a motion inside the solvation shell. This idea is used to build a theory that predicts appearance of many ion sizes with enhanced diffusivity. This result is also confirmed by molecular dynamics simulation of ion diffusion in liquid xenon and water. Effects of the system size and incorrect liquid viscosity are taken into account. The results are shown to be independent of the interaction potential model. The results are found to be in a good agreement with experimental data on ion diffusivity in water and liquid xenon. The abstract was prepared within the framework of the Basic Research Program at the National Research University Higher School of Economics (HSE) and supported within the framework of a subsidy by the Russian Academic Excellence Project “5-100”.

On distribution of particles over the constituent clusters

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The universal distribution function of particles over the constituent clusters have been established (see also [1]). This distribution should be distinguished from the distribution of clusters over the comprising particles (i.e. over the cluster sizes). The connection between both distributions has been established. It has been demonstrated that the former one is more reasonable for use if the system consists of relatively small number of big clusters, i.e., for example, if system is close to its condensation conditions. The proposed distribution is universal in the sense that its form depends on a single parameter, which is $\eta = a/l_0$, where $l_0 = 0.55n^{-1/3}$ is the mean distance between particles, which assumed to randomly distributed over the whole volume, and a is the “interaction radius”. “Particles” in this model are non-interacting spheres. We assume that two particles belong to the same cluster if the distance between them does not exceed the “interaction radius” of this sphere a . The results have been compared with well known distributions. It turns out that in the region of small cluster sizes the universal distribution coincides with Kolmogorov log-normal distribution [2].

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Intercalation of graphite and graphene-like structures by metal atoms and its study by vibrational spectroscopy

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Metal-graphite intercalation compounds M-GIC have intercalated layers with a lacunar structure in which it is possible to accumulate large quantities of metal and metal compounds. The reason is that interlayer distance in M-GIC is much larger than in ordinary graphite monocrystal. For an example interlayer distance in M-GIC changes from $d = 5.40$ to 5.69 [1], whereas in graphite it is 3.35 . Intercalation of graphite by metal atoms have been carried out by the two-zone vapour transport method. We have fulfilled simulation of M-GIC metal atoms capacity for different intercalation stages. Lattice dynamic for M-GIC have been studied by means of Raman scattering spectroscopy with on LAMMPS program with using of Tersoff, ReaxFF and REBO many atoms potentials [1]. This work is supported by the Russian Science Foundation (No. 16-29-13011).

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The use of low-background nuclear spectrometry for the study of metal graphite intercalation compounds and multilayer graphene

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The objects of our study are metal graphite intercalation compounds and multilayer graphene intercalated by alkali metal atoms. The degree of potassium atoms intercalation of multilayer graphene samples will be studied by the method of thermal programmed desorption of the radioactive isotope ⁴⁰K under low background conditions [1]. Methods of positron-annihilation spectroscopy have been used for Fermi surface reconstruction by means of Doppler broadening and anisotropy of the distribution of annihilation photon pair momenta. For determination of the cavities sizes and the types of atomic vacancies positron annihilation lifetime spectroscopy was realized. The possibilities of applying Mossbauer spectroscopy for iron-graphite intercalation compounds study discussed for iron enriched by isotope ⁵⁷F. This work is supported by the Russian Science Foundation (No. 16-29-13011).

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Liquid drop model of nuclei capillary oscillations with account of viscosity

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Liquid drop model (LDM) successfully being used for semi-empirical formulation of surface and Coulomb terms in Bethe–Weizsacker mass formula. In this study in the frame of nuclear liquid drop model an analytical solution for the frequency of capillary oscillations is obtained with taking into account the damping due to viscosity and surrounding medium motion and polarizability. Comparison of quadrupole and octupole vibration frequencies gives for nuclei matter viscosity [1]:

$$\eta = \rho a^2 \sqrt{\frac{15\omega_2^2 - 4\omega_3^2 + (60E_c)/(7Ma^2)}{784}}, \quad E_c = \frac{3}{5} \frac{Z^2 e^2}{a},$$

where a is nucleus radius, ρ is the nuclear matter density, ω_2 and ω_3 are the quadrupole and octupole frequencies correspondently. The model has been applied for estimation of spherical nuclei surface tension and viscosity [2]. Experimental data analyses give viscosities in the interval $4.2\text{--}7.6 \text{ MeV fm}^{-2} \text{ s}^{-1}$ for nuclei from ^{106}Pd to ^{198}Hg . It is shown that as the temperature increases, the process of buildup of quadrupole and octupole oscillations amplitudes leading to the nuclei decay of into two and three fragments, respectively.

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The glass transition criteria

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Molecular dynamics study of the glass transition is performed. As an example, the Al–Cu melt is taken. There are several glass transition criteria: the decrease of the specific heat of material (calorimetric criterion), the splitting of the second peak of the pair correlation function and the icosahedral short-range order (structural criteria), the change of diffusivity behavior (dynamic criterion). The difference between the calorimetric glass transition temperature and the temperature, obtained using the structural and dynamic criteria might reach several hundred kelvins [1]. In the current work we obtain the glass transition temperature using two methods based on the shear stress correlations behavior. The first method is based on the stress correlations in the plane of the film and the steep change of the kinematic viscosity. The second method is based on the transverse oscillations in the film. The glass transition temperature is estimated from the temperature dependence of the oscillation damping of the stress correlation functions. The increasing in the kinematic viscosity correlates with the decrease of transverse oscillations damping in the film [2]. The authors acknowledge the Supercomputer Center of Joint Institute for High Temperatures RAS and Joint Supercomputer Center RAS for providing computing time. The work is prepared within the framework of the basic research program at Higher School of Economics and supported within the framework of a subsidy by the Russian Academic Excellence Project “5-100”.

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Collective effects and liquid–glass transition in supercooled melts of binary alloys

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We discuss results of the method of spatial correlation functions [1] to find any kind of collective motions suchlike discussed in [2]. In the proposal to check the effect of transition on the behavior of some thermodynamic functions in supercooled liquids, we used a system of the glass-forming liquid of some alloys melts in different phase states. It was found that some correlators sharply change the nature of their time dependence when the melt is supercooled. After making physical interpretations, we considered using some of these changes in the different 4-point spatial functions [3] as manifestations of transition into metastable or glass state. Finally, we analyze differences in behavior of spatial functions for models of alloys with various compounds. Comparison with other results of phase transition in taken alloys is also given. All new data have been calculated by performing molecular dynamics simulations. This work was supported by grant of the President of Russian Federation for young scientists MK-1404.2017.8. The authors acknowledge the Supercomputer Centres of JIHT RAS and MIPT for providing computing time.

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Viscosity of hydrocarbon mixtures in liquid state

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We present a study of viscosities of methane, n-butane and their mixtures by the non-equilibrium molecular dynamics simulations and empirical correlations. The hydrocarbons are simulated in the TraPPE-EH force field [1]. The viscosities of pure components are found to agree with the Batchinski equation in a wide pressure range. The viscosities of mixtures can also be described by the Batchinski equation. The Batchinski parameters for mixtures can be found by linear mixing of the respective parameters for pure components. Widely used cubic root and Arrhenius mixing rules are also tested for the mixture viscosities. To calculate pure component viscosities, we used the Batchinski equation and the concept of molecular volume of component in mixture based on the Voronoi tessellation. Both cubic root and Arrhenius mixing rules systematically underpredict mixture viscosities. Generally, Arrhenius mixing rule gives lower viscosities than cubic root mixing rule. The predictions of the model with Batchinski mixing are in good agreement with the bubble-point line liquid viscosities reported in literature [2]. The abstract was prepared within the framework of the Basic Research Program at the National Research University Higher School of Economics (HSE) and supported within the framework of a subsidy by the Russian Academic Excellence Project “5-100”.

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The non-equilibrium molecular dynamics calculation of methane viscosity in the COMPASS force field

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The transport properties of hydrocarbons and their mixtures are of great applied interest in the oil and gas extraction industry. The simulations of extraction processes and flows in porous media require models for prediction of viscosities of liquid and gas phases. In this work, the properties of liquid methane CH₄ and its mixtures with different hydrocarbons are studied using classical molecular dynamics (MD) methods. The interatomic potential is COMPASS [1]. The shear viscosity is calculated using non-equilibrium MD [2, 3]. The temperature range is from 300 to 360 K. The pressures are varied from 500 to 10000 atm. The results calculated using COMPASS force field are compared with the values predicted by the TraPPE-EH [4] force field in the previous work. The TraPPE-EH potential has simpler model of interaction between atoms. The predictive power of both potentials is analyzed. The calculations are performed in the LAMMPS package. The authors acknowledge the Joint Supercomputer Centre of RAS and the Supercomputer Centre of the JIHT RAS for providing computing time. The article chapter was prepared within the framework of the basic research program at the HSE and supported within the framework of a subsidy by the Russian Academic Excellence Project “5-100”.

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Investigation of the liquid and gas densities on the saturation line: Some scaling models and numerical data in the critical region of H₂O and SF₆

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We make an analysis of some literary sources. The sources describe the liquid density (ρ_l) and the gas density (ρ_g), which are related to the saturation line in the critical region of H₂O and SF₆. In the analysis, we have considered analytical forms of (i) equations of state among them a formulation (IF-95) and recommended by IAPWS as well as (ii) $\rho_l(\tau)$ and $\rho_g(\tau)$ equations among them Anisimov model (1990, 2007) those are valid in a narrow temperature interval, $\tau = 0.002-0.012$. Here, $\tau = (T_c - T)/T_c$ is a relative temperature. We pay an attention to a scaling model, $F(\tau, D, C)$. The model is related to a row of properties (ρ_l, ρ_g, f_d, f_s) and follows to the scale theory of critical phenomena, here $D = (\alpha, \beta, T_c, \rho_c, \dots)$ are critical characteristics, α, β are indexes, C are adjustable coefficients, $f_d = (\rho_l + \rho_g)(2\rho_c)^{-1} - 1$ is the mean diameter, $f_s = (\rho_l - \rho_g)(2\rho_c)^{-1}$ is the order parameter. An Anisimov model, $f_d(\tau, D, C)$, is investigated. A combined scaling model is elaborated in the work. This model has a modern structure and meets the scaling theory. We have got $\rho_l(T)$ and $\rho_g(T)$ equations on the base of the combined scaling model. Our analysis shows that these equations satisfactorily reproduce data on ρ_g and ρ_l, T in a wide temperature interval. Thus, there is a good agreement of $\rho_l(T), \rho_g(T)$ models for H₂O with data included in tables (IF-97) and valid in the interval, $\tau = 0.002-0.2$.

Fundamental equation of state for argon

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In this work, an equation of state (EOS) is developed in the form of the Helmholtz free energy, $F(\rho, T) = F_r(\rho, T) + \phi(\rho, T)F_n(\rho, T)$, where $F_r(\rho, T)$ and $F_n(\rho, T)$ are the regular and non regular density ρ and temperature T functions, respectively; $\phi(\rho, T)$ is the crossover function. The EOS is to represent experimental thermodynamic data of argon in the regular and non regular, critical, region. The non regular addend, $F_n(\rho, T, D)$, is built in accordance scaling theory (ST). This EOS includes such parameters as critical characteristics, $D = (\alpha, \beta, \dots)$, that are proposed by ST and connected with singularities of thermodynamic properties in the critical point. The component $F_n(\rho, T, D)$ of the EOS is developed on the basis of a new presentation of the scale and the Benedek's hypothesis [1]. The proposed approach is similar to the method considered in [2]. Experimental (P, ρ, T) data and (C_v, ρ, T) results (Anisimov A M *et al* and Voronel A V *et al*) of argon are combined in an input data set. It is placed in the T, P intervals: 83.8–1300 K and 0.01–1000 MPa. A fitting routine is used to treat (P, ρ, T) data together with (C_v, ρ, T) results for the purpose of determining the EOS coefficients. A software program is produced for the calculation of thermodynamic properties with the help of the EOS. Calculated data are compared with experimental results as well as with known tabulated properties and equations of state [3–6].

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Method of construction of an equation of state consisting of a scale hypothesis

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The presented method of constructing the fundamental equation of state (EOS) is based on the following expression for the Helmholtz free energy $F(\rho, T)$:

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

Here the scale function $a(x)$ is calculated in the framework of the following concept of a large-scale hypothesis:

$$\Delta\mu(C_V/T)^{\beta\delta/\alpha} = \varphi_1 m + \varphi_2 m^3, \quad m = \Delta\rho(C_V/T)^{\beta/\alpha}, \quad (2)$$

where $\Delta\mu = (\rho_c/p_c)[\mu(\rho, T) - \mu_0(T)]$; μ is the chemical potential; $\Delta\rho = \omega - 1$; $\omega = \rho/\rho_c$; α, β, δ are critical indices; C_V is isochoric heat capacity; x is scale variable.

On the basis of the fundamental equation (1) EOSs for R1234yf, R218, R32 have been developed which in the regular domain of the thermodynamic surface satisfy all the requirements imposed on the equations of state of the virial species. It is shown that in the neighborhood of the critical point and in the regular part of the thermodynamic surface (including the region of dense liquid and high pressures), the proposed EOS, firstly, satisfies the scale hypothesis, and secondly, with a small error, experimental data on the equilibrium properties of the investigated substances.

Continuum filtration model of two-component hydrocarbon system

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The work is dedicated to realization of filtration model. Thermodynamics of the model is based on Brusylovsky equation of state (EOS), the aim of it is to find phase equilibrium. Hydrodynamics consist of two mass conservation equations (one for each phase: liquid and gas).

Mathematical modeling of pulsation filtration regimes of gas-condensate mixtures taking into account nonequilibrium phase transitions

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The present work is devoted to mathematical modeling of the wave filtration process. It is shown that periodic solutions can arise in the retrograde region of the phase diagram. The article shows the existence of a pulsational character of the filtration regime of the flow of a hydrocarbon mixture, the occurrence of which in practice can be explained by the constant inflow of heavy components into the bottomhole zone, and then by their condensation, which leads to an increase in the volume of the liquid phase. Further, when a sufficient amount of liquid is accumulated and its mobility increases, it comes to the well, the saturation profile flattens out and the process repeats. The solution of the system of differential equations for the filtration of a gas-condensate mixture in a porous medium taking into account the nonequilibrium of phase transitions is made by the finite element method in the FlexPDE package. This work was supported by the Russian Science Foundation (project No. 14-50-00124).

Physical simulation of the filtration process of the methane–n-butane mixture

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Experimental studies of various filtration regimes of the model gas-condensate mixture “methane–n-butane” were carried out under full-scale thermobaric conditions. It is shown that the presence of a retrograde region on the phase diagram of this mixture can significantly affect the character of the hydrocarbon fluid flow. The conditions for the appearance of the “liquid plug” regime are determined, in which the retrograde liquid prevents the fluid from moving through the porous medium.

This work is supported by Russian Foundation for Basic Research (project No. 17-08-01270).

2. Shock Waves, Detonation and Combustion

Investigation into shock compression of the materials

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Shock-waves are the basic tool for reaching extreme states of matter. In RFNC-VNIITF, we use explosive measuring of flat, cylindrical, and spherical geometry as well as gun-type accelerating devices for shock-wave generation. State-of-the-art dynamic measurement methods, based on various physical phenomena and principles, are used to register extreme states of matter.

It is due to the development of nuclear arms that the physics of extreme states of matter was created, because shock-waves play the role of preparatory mechanism for chain reaction. In its turn creation of nuclear charges promoted investigation into physical processes taking place under conditions that have never been reached in laboratory environment before. Due to this, various properties of matter, including shock compression, were investigated almost since when the first experiments aimed at measuring explosion parameters were conducted.

In this work we review the methods of studying materials compressibility including loading methods and shock-wave processes registration methods, used in RFNC-VNIITF for the benefit of explosion physics and physics of extreme states of matter.

Dynamic registration of ejection from shock-loaded metals

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When a strong shock wave in the metal out on the border with air, from the surface is the release of microparticles. The phenomenon encountered in the measurement of the speed of the foil (glued to the explosive charge) using VISAR. Interest in this phenomenon is also associated with the development of instability and strength of materials in micro and nanoscale. Most experimental studies aimed at studying the ejection of particles from the shape and size of discontinuities (notches, grooves) on the surface of metals. The obtained data required for numerical simulation of emission of particles. In this work, the mass distribution along the jet was measured simultaneously by the piezoelectric transducer and x-rays using a soft spectrum of synchrotron radiation of the Collider VEPP-3. This work was supported by Russian Foundation for Basic Research (No. 16-29-01050)

Hugoniot of porous Ni–Al reactive mixture samples of different dispersity

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A study of the possibility of a fast reaction in Ni–Al equiatomic mixture samples at shock compression before unloading was conducted. Two types of samples were used: samples prepared of microdisperse (low reactivity) and nanodisperse (high reactivity) mixtures. The porosity of samples was about 25%. The Hugoniot measurements were fulfilled up to 60 GPa. Equation of state of the samples was constructed. Location of the Hugoniot relatively to melting lines of the components is estimated. The loading of the samples was carried out using explosive throwing devices. The registration of velocity profiles on the boundary sample-water window was performed using VISAR. Shock velocity was determined by time markers. It was found that the profiles did not reflect noticeable signs of possible reaction between the components. The coincidence within the experimental error of Hugoniot for both types of the samples despite significantly different dispersity of components was revealed, which indicates a complete chemical transformation, or its total absence. At the same time, the Hugoniot, estimated using the equation of state without taking into account the reaction between the components passes in close proximity to experimental, which rather points to the lack of reaction. Assessment of the relative position of experimental Hugoniot and melting lines of the components shows that for a given porosity of samples, melting of aluminum, which is more refractory than nickel at high pressure, may begin near 60 GPa.

Experimental study of dynamic properties of microspheres-containing silicon rubber under shock-wave loading

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The work is devoted to the study of shock-wave properties of porous materials. Porous media, by the example of silicon rubber with glass microspheres, were chosen as the objects of the investigation. In the first case, we used calibrated microspheres, featuring average size of 80 μm . In the second case, the size of the microspheres varied within the range from 20 to 150 μm . Free surface velocity profiles of the loaded samples were obtained with VISAR laser Doppler velocimeter. The investigated samples feature specific, rather complicated structure of the shock-wave front. First, there was registered a two-wave configuration. Second, there were observed noticeable oscillations of the velocity profiles behind the shock jump. Processing of the experimental data resulted in creating the Hugoniot of the investigated materials. The porous materials in question were investigated at low pressures; there were obtained negative-curvature isentropes, their negative curvature being caused by the kinetics of the pores collapse. Also the investigation of spall strength value and its relation to the strain rate were facilitated. The work is carried out with the financial support of FAIR—Russia Research Center.

Experimental investigation of epoxy resin under shock waves

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Using a light gas gun and high explosive generators for acceleration of aluminum plates, the experiments for determination of Hugoniot, the shock wave structure and spall strength in epoxy resin were conducted. The density of the samples is 1.2 g/cc, the measured sound speed is $c = 2.63$ km/s. Shock wave profiles were recorded by a laser interferometer VISAR and PDV with the use of 8 channels. In each experiment the structure of compression pulse and the shock wave velocity of epoxy resin were obtained. Pressure of shock compression varied by changing of the thickness and the velocity of projectiles. The projectile velocity varied from 165 up to 2500 m/s. At low pressures of incoming pulse to the samples after the shock jump there is an increase of velocity during $0.5 \mu\text{s}$, what is connected with relaxation processes in the compression wave. At high pressures relaxation is not observed and after the shock jump the value of particle velocity is constant. From the experimental data Hugoniot of epoxy resin was obtained. At high pressures it can be approximated by a linear dependence of $D = 2.6 + 1.18u$, km/s. Also the spall strength was investigated. Its value changes from 280 up to 360 MPa, when the strain rate varies from 1.2×10^4 to 7.2×10^4 1/s.

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

Polymethylmethacrylate double compression registration using synchrotron radiation

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Experiments with single and double shock compression of the materials provide background for the development of equation of state (EOS) of the material under high pressure. Double compression compared to single compression provides smaller growth of the internal energy, the states that occur due to this phenomenon are observed below Hugoniot curve, approaching to isotherm. The fact helps to understand the value of the experiments with double compression conducted in order to investigate into the states of matter and its EOS under high pressures.

The work describes the setup and results of the experiments where two modes of shock-wave collision were observed. Synchrotron radiation was used to register processes of incident shock wave propagation and collision, as well as reflected shock wave formation. The experiments were conducted using accelerator of the Budker Institute of Nuclear Physics SB RAS.

Interaction of blast waves with helium-filled rubber balloons

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Gas-filled elastic bags are a convenient means for storing blast mitigation materials, such as inert gases and two-phase media, and delivering them to protected objects. If the blast wave resulting from an accident propagates through air, it can undergo significant transformations when interacting with various inhomogeneities. This study explores the possibility of blast-wave attenuation by interaction with a thin enclosure (shell) filled with helium, which has a low specific acoustic impedance compared to air. Experiments are conducted in a vertical shock tube having a diameter of 54 mm and a length of 1.5 m. Blast loads are produced by deflagration-to-detonation transition of a 35% hydrogen-in-air mixture in the tube section containing ring obstacles. The tube is filled by blowing the mixture through it. The ignition source is in the top section of the tube. The open bottom of the tube has a short flared section designed to reduce the wave attenuation due to transverse expansion. Helium-filled rubber balloons are placed on the test plate located at a distance of 150 mm from the tube exit and equipped with pressure sensors. High-speed shadow photography is used to investigate the wave patterns and dynamics of helium compression in the balloons under blast loads resulting from explosions of hydrogen-air mixtures. Blast loads transferred to the test plate are analyzed. A comparison with 3D numerical simulations shows that the motion of a thin shell can be computed by solving fluid dynamics equations without specifying boundary conditions across the shell.

Structural changes of calcite after shock treatment in the Mbar-range

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Shock experiments in the pressure range up to the Mbar-boundary, concerning carbonates, were mostly restricted up to present date to the behavior of carbonate rich rocks during large impact events. This may explained by its rapid degassing along the release path after shock experiments although these compositions are stable also under high pressures [1]. The novel developments of the Freiberg High Pressure Research Centre (FHP) opens now the new research field far beyond the current borders (approximately 60 GPa [2]) for the investigation of carbonates after shock treatment up to 2 Mbar without any degassing reactions. This involves both phase transitions into unusual carbonate structures and intense twinning and plastic deformation. For these investigations also the loading with multiple reverberations must take into account.

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Structural changes of cristobalite under dynamic and static pressures

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In this work the structural changes of cristobalite under the influence of high dynamic and static pressures were investigated. To create high dynamic pressures the samples were loaded by high temperature shock compression method similar that used in [1]. According to the method the samples put in copper ampoules were shock compressed using planar loading scheme. Shock waves were generated by aluminum plates accelerated with detonation products of various explosives to several km/s. Depending on experimental setup and explosive used pressure in samples were 14–37 GPa. Studies under static pressure (8 GPa) were carried out in toroid-type apparatus. After carrying out shock-wave and static experiments, the extracted samples, if necessary, were purified by boiling in acids. Then the samples were investigated by powder x-ray diffraction. New non cristobalite peaks were fixed on the diffractogram of cristobalite loaded to 14–28 GPa. The Rietveld analysis showed that the obtained diffractograms did not correspond to the structure of the original cristobalite. Comparison of x-ray diffraction patterns with x-ray diffraction data for other silica phases also showed no correspondence, i.e. one can talk about transformation of cristobalite into a new phase. Amorphization of cristobalite occur at a higher dynamic pressure. Experiments at static pressure confirm the formation of a new phase of silica under the dynamic loading. Analysis of the x-ray patterns of the new phase suggests that the structural changes of cristobalite are phase transformations without radical restructuring and changing the coordination number.

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On the existence of polymorphic transitions in high-purity titanium BT1-00 according to the results of sound velocity measurements

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Here results of the sound velocity measurements in shock-compressed high-purity titanium BT1-00 (in accordance with GOST 19807-91) in the pressure range up to 170 GPa are present. Processes were registered using photoelectric method [1, 2] in experimental setup with overtaking rarefaction wave. According to experimental data obtained the material is in solid phase at considered pressures. Calculation and theoretical analysis [3] reveals that shock-wave melting starts at 150 GPa. The fact that the polymorphic transformation takes place at 50–60 GPa is verified, which agrees with calculation and theoretical assessments [3]. The fact of transition is evidenced in the work [4] but pressure range of transition in that work is somewhat higher compared to the results of this work.

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Equations of state, equilibrium lines and conductivity of polymorphous modifications of hafnium at high pressures

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Hafnium is an important material of the nuclear industry. The main functional feature of this metal is the ability to absorb thermal neutrons. Study hafnium properties under high static and dynamic pressures many papers. However, in the scientific literature on hafnium, there are contradictions regarding the location and slope of the equilibrium lines in the phase diagram. Therefore, the phase diagram needs to be supplemented and refined by experimental methods.

In this paper, experimental data are obtained on the electrical conductivity and thermophysical properties of hafnium in the region of extreme states, where structural transformations and accompanying changes in the electrophysical properties of this material occur.

The equations of state of polymorphic modifications— α , ω and β phases of hafnium are developed and mathematical modeling of the experiments. The equilibrium lines of $\alpha \leftrightarrow \omega$, $\omega \leftrightarrow \beta$ and $\alpha \leftrightarrow \beta$ phases are calculated and, thus, a phase diagram of hafnium is constructed in the region of existence of high-pressure phases of hafnium up to pressures of 80 GPa and temperatures up to 2000 K. The electrical resistivity of hafnium samples was measured up to pressures of 140 GPa in conditions of step shock compression. Experimental data have been obtained on the electrical resistivity of the α -phase of hafnium in the pressure range up to 40 GPa and temperatures up to 1300 K.

The behavior of chromium and molybdenum under ultrafast loading

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In the present work, the interaction of a long load with a steep front on refractory metals was considered. The influence of a short laser pulse on a submicron thickness target was investigated. For the study an interferometric measurement technique was used using a frequency-modulated (chirped) diagnostic pulse. As a result of the experiments it was recorded splitting of the shock wave into elastic and plastic. During the experiment loads were created that made it possible to obtain pressure behind the front of the shock wave to 20 GPa. The dynamic strength of metals in a solid state under a load of about 20 ps was studied in detail.

Dynamic tensile strength of liquids lead–bismuth eutectic, lead and tin under shock-wave loading

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The problem of the dynamic strength of metallic melts appears in analysis of the operation of liquid-metal heat carriers of promising pulsed power facilities, calculations of the operation of meteorite protective shields of spacecrafts, analysis of the kinetics of the nucleation and growth of a vapor phase, and in other similar problems. In the submicrosecond range of load durations, the tensile strength of solids and liquids is determined by analyzing spalling phenomena appearing at the reflection of a compression pulse from the free surface of a sample. In this case, fracture stresses at spallation are determined by analyzing the measured free surface velocity history by the method of characteristics.

The dynamic tensile strength (spall strength) of lead–bismuth alloy, tin and lead melts has been measured by a found method. Comparison with similar measurements of the spall strength of these metals at room temperature shows that melting reduces the spall strength by at least an order of magnitude. The spall strength of liquid metals is a smaller fraction of the extremely possible (“ideal”) strength than that for water and organic liquids.

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

VISAR-measuring profiles of the average mass velocity in the propagation of the shock wave compression in spheroplastic

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Laser interferometer VISAR was applied for investigation of shock compression waves in epoxy compounds modeling emulsion substance. The volume fraction of the glass microspheres in the epoxy compound was 0.7. The glass microspheres diameters were of 20 to 80 μm . Powder gun caliber 57 mm was used to throw plane impactors of the aluminum alloy. The velocity profiles of the free surface of compound samples were obtained at the impactor velocity region of 350 to 580 m/s. Found to be the free surface velocity profiles of spheroplastic had a two steps shape unlike one step shape in the homogeneous compound. The dependence of free surface velocity raise time versus impactor velocity was obtained. The work was supported by Presidium RAS.

Stability of relativistic shock waves: Theory and numerical experiment

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The nonlinear analysis of the shock waves unstable in accordance with linear stability theory criteria [1] is extended to relativistic shock waves. The analysis is based on numerical solution of initial value problem for the relativistic hydrodynamics equations with initial data corresponding to the unstable shock wave. The model equation of state used in the numerical experiments is compatible with relativistic theory (does not produce superluminal speed of sound) and meets to the requirements of thermodynamic stability. The Hugoniot–Taub adiabats for the model equation of state contain segments in which the shock waves are unstable in accordance with stability theory of relativistic shock waves [2–6]. The equation of state with required properties is developed on the basis of model equation of state [7]. Ambiguity of the shock-wave discontinuity representation in these segments determines the character of the shock wave behavior: one-dimensional splitting with formation of a composite compression wave or two-dimensional splitting based non-stationary mode. This behavior is shown to be analogous to the case of non-relativistic shock waves violating stability criteria. Fulfillment of the shock wave instability criteria for the case of relativistic shock waves in nuclear matter is discussed.

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Study of multiple spallations in flat metal plates made of 12H18N10T austenitic steel by recording velocity profiles and axial stresses in marble barrier using two independent measurement techniques

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The paper presents results of explosive experiments with concurrent recording of signals from four low-resistance gauges and three interferometric laser velocimeters. The objective is to test experimentally the predictions and results of recording gas-dynamics processes using two independent techniques: multichannel manganin (MDD) and laser-interferometry based on laser heterodyne (LHM). The task is to obtain, in addition to performed calculations and earlier experiments, the results of measuring $s_{xx}(t)$ in real physical process with double artificial spall in the impactor made of 12H18N10T steel; to measure the velocity $w(t)$ of the first plate and to record the velocity profile of 12H18N10T—window material (LiF) boundary under impact of all flying cascade. The plane-wave loading device, the recording techniques, that is, manganin gauges and laser heterodyne, are described, the design and composition of used mechanical assembly (impactor material and quantity, their density and thickness, flight route, material and thickness of target elements) are presented.

Two-level models of dynamic plasticity and fracture of magnesium

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Magnesium and magnesium alloys attract increasing attention as lightweight structural materials with high specific strength. Appropriate models of plasticity and fracture of such materials are necessary parts for complete the description of its behavior in addition to the equation of state. Structural models considering evolution of structural defects have obvious advantages in possibility to take into account the initial microstructure and to be valid in a substantially wide range of loading parameters including dynamical regimes with high strain rates. Higher number of parameters can be partially reduced by application of atomistic simulation for their determination as these parameters typically have clear physical meaning.

Earlier we developed structural models of plasticity and fracture of several metals using two-level approach. Here we present their modification for the case of magnesium single crystals. The plasticity model is developed to take into account the crystal anisotropy and the finite deformations. Thermodynamic consistency of the model is discussed. On the atomic level, the molecular dynamic (MD) simulations are used to determine the dislocation motion equation and corresponding parameters, as well as the temperature and pressure dependences of the elastic modules. The obtained data are used on the continuum level to close the plasticity model. The fracture model is developed to take into account the anisotropy of magnesium single crystal; it is also based on MD simulations. The models are verified by comparison with the literature experimental data for the high velocity plate impact.

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Influence of local stresses on motion of dislocations

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Based on the theoretical consideration and analysis of molecular dynamic (MD) simulation data, we show that the dislocation motion is determined by the stress field in its local environment. These stresses differ from the values averaged over even such tiny microscopic regions, which are usually used in MD study of dislocation motion. As a result, the slip velocity of dislocations can remain virtually constant with a gradual decrease in the average stresses in the calculation area. When a dislocation enters the trace of the previous dislocation, that is, into a region plastically relaxed by the slip of the previous dislocation, its velocity, on the contrary, decreases sharply, even if the average stresses in the region vary slightly. The revealed complex behavior leads to variable final average stress after the completion of the movement of dislocations; the average stress sometimes even changes its sign in the course of plastic relaxation. All these features can influence the response of the dislocation system to mechanical loading. Therefore, the action of the local stresses should be taken into account when analyzing the MD results, in the development of continuum models of plasticity, as well as in discrete dislocation dynamics. A dislocation motion equation is proposed with accounting of local stresses, and the constants for the edge dislocation in Al are determined by comparison with the results of MD simulations. An asymptotic solution of this equation is proposed, which can be used in the numerical solution of the equations of continuum dislocation plasticity. Alternative dependencies of the drag force on the dislocation velocity are analyzed; it is shown that they describe the results of MD simulations worse than the equation proposed by us.

Research nucleation dislocation from grain boundaries in aluminum bicrystals

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This investigation is analyzed dislocation structure in aluminum bicrystal during shear strain using molecular dynamic (MD). MD is performed with LAMMPS, for visualization used OVITO and the atomic interaction is described with the help of embedded atom potential. Bicrystals are builded using Voronoi method in Atomsk software package. This 13 crystal with various symmetric tilt angle (0 (monocrystal)–40.316) and [110], $[\bar{1}10]$, [001] crystallographic direction are modeled. They samples consist from 503520 to 523520 atoms. Analysis of results shows 3 types grain boundary (GB) in this range angle: (i) typical low-angle GB; (ii) undefined structure in 2 samples; (iii) GB consists of Frank dislocations in high angle tilt. For type 3 GB motion is not happening. Monotone dependence between tilt angle and dislocation is not observed. Furthermore, the slip plane Shockley dislocations are different: with increase angle misorientation involved slip system that projection on the shear direction is grows. In this work shear stress is depend dislocation nucleation, that is consistent with [1]. It stress decreases with misorientation angle grows. In summary, this investigation shows dislocation nucleation factor in bicrystal: GB structure (such as [2]), the slip system dislocation Shockley changing, GB energy. The work is supported by the Ministry of Education and Science of the Russian Federation, state task No. 3.2510.2017/PP.

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Plastic deformation of metal nanoparticles under shock wave compression

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Shock-wave action is often used to compact the nanopowder. The application of molecular dynamics modeling allows us to consider the details of this process for the case of nanoscale metal particles. The picosecond compression pulses are carried out by successive pressure pulses to the front surface of the test sample. The interaction of the shock wave with the deposited nanoparticles on the substrate leads to plastic deformation in the surface layer of the metal. The presence of precipitated nanoparticles on the rear surface increases the threshold value of the impact intensity leading to the rear spall. The dislocation density, shear deformation under plastic deformation of metal nanoparticles are considered.

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

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With high-speed dynamic loading, it is possible to destroy materials, for example, a splitting of the rear surface at the exit on it to the shock wave. The process of destruction consists of the nucleation and growth of pores. Which eventually lead to formation of cracks and tearing of the material. The standard mechanism of pore growth is realized through the nucleation and movement of dislocations on the pore surface [1, 2].

In paper [3], the authors proposed a model of dislocation-stimulated growth of nanopores in aluminum in order to predict the critical tensile pressure in the volume of a substance containing a nanopore. Molecular dynamic simulations were used to verify the proposed continuum model and to fit their parameters. Here we continue this work and apply the proposed model [3] to the case of copper. In the work, the results of molecular dynamic simulations in comparison with the continuum model are presented.

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Growth of voids in magnesium and its fracture at tension

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One of the most perspective materials for the use in the aerospace and automotive industry, in the creation of mobile electronic devices, as well as in biomedical applications is magnesium and its alloys. On the one hand magnesium and magnesium alloys have a smaller specific weight, and this offers the challenge for its use in various applications. On the other hand, the use of magnesium and its alloys is limited by the relatively low mechanical strength. Therefore, investigation of mechanisms for the fracture of magnesium, the effect of inclusions and pores on its strength is an urgent task.

With the help of molecular dynamic simulation, we investigated the growth of pores in magnesium and its fracture under tension. Studies of uniaxial tension of magnesium, magnesium with pore and magnesium with aluminum inclusion along different axes were made. The tensile strength of systems is determined at varied strain rates (in the range from 0.1 to 10 ns⁻¹ at the temperature 300 K) and varied temperatures (in the range from 300 to 1100 K at the strain rate 1 ns⁻¹). The rate sensitivity of strength of a material with inclusions is higher than that for a material without inclusions.

We propose a continuum model of fracture, taking into account magnesium anisotropy, which is based on the equations of nucleation and growth of voids; the model takes into account the stress concentration around inclusions. A comparison with the MD results shows that the continuum model allows us to describe the rate and temperature dependences of strength at least for strain rates 0.1 ns⁻¹.

Modeling of cylindrical shell collapse in finite deformations

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Experiments on collapse of cylindrical [1] and spherical metal shells are used for researching the deformation behavior of metals in the conditions of energy accumulation in the converging shock wave. A significant experimental material has been accumulated currently. Earlier, we already simulated the process of cylinder collapse with using models of fracture and plasticity. In this work, equations of state and equations of plastic deformations are generalized for the formalism of finite deformations, because the values of deformations in the problem of cylindrical aluminum shells can be more than one. Continuum mechanics equations are solved numerically in the one-dimensional cylindrical formulations with using the numerical method [2]; the substance behavior is described by using the of dislocation plasticity model [3, 4]. The work is supported by the Ministry of Education and Science of the Russian Federation, state task No. 3.2510.2017/PP.

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The output of a shock wave on the inner surface of a cylindrical liner

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The authors have previously performed experimental study and mathematic simulation for cylindrical detonation wave. The results are presented in the works [1,2]. Further research has found some specific details on the surface of cylindrical detonation wave formed by the multipoint initiation method, as well as peculiar gas dynamics of detonation products flow. Multipoint initiation method can be applied for metal plates acceleration and cylindrical, conical or spherical shells compression. Herewith as a strong shock wave reaches free surface of the compressed metal liner, it causes fine particles and plasma emission [3]. The paper considers experimental recording of the surface physical property. When a shock wave created by detonation wave, formed by the multipoint initiation method and characterized by presence of “nodes” and “bundles” (bright bands), reaches free surface of the liner, not only plasma and fine particles flow is formed, but also liner structure can collapse because of local pressure jumps in the “nodes” that form a grid in accordance with initiation points arrangement. The article is concerned with this phenomenon study. It presents the results of high-speed photography during large-scale experiments and experimental results obtained by means of a laboratory setup earlier adjusted at the Institute of Problems of Chemical Physics of Russian Academy of Sciences (IPCP RAS).

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Gasdynamic generators of the pressure pulse

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Gasdynamic devices are traditionally used for time-dependent loadings at strength tests of constructions [1–3]. The method of the sliding detonation of sheet explosive is used often when strength tests are carried out to pulse loadings. The main defect of this method is nonsimultaneity of the action of loadings localized in different points of the construction. Failure of a detonation appears additional difficulty at a small thickness of an explosive. In the present work the set of gasdynamic devices allowing to generate low-pulse loadings is considered. Considerable attention is paid to achievement of high simultaneity of action of loadings generated in various points of the construction. The simultaneity is reached by the original systems of initiation of the explosive distributed on a construction surface. Results of validation of modern devices for generation of pressure impulses are given. The considered set of devices is used for strength tests of constructions when action of the energy fluxes [4] takes place. Work is made with support of the Russian Foundation for Basic Research (project No. 16-08-01065).

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Superconductivity of shock-wave pressure treated Na–WO₃ mixture

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Tungsten oxide WO₃ is a semiconducting material consisting of WO₆ octahedrons, which can connect together in various ways, leading to a large multiplicity of the WO₃ crystal structures. The structural interstices located in between the interconnected WO₆ octahedrons allow the intercalation of WO₃, resulting in formation of so-called tungsten bronzes M_xWO₃, where M is an intercalant ion that donates electrons to the WO₃ host matrix. Since the discovery of superconductivity in tungsten bronzes these superconductors are attractive up to the present time. Here we report on the superconductivity at $T_c = 40$ K of the samples prepared by the shock-wave pressure (about 20 kbar) treatment of the NaWO₃ mixture of 1 : 1 molar ratio. The samples were prepared with applying the flat-type shock-wave pressure setup. The starting material was tablets, 10 mm in diameter and 3 mm thick, prepared of 1 : 1 molar ratio mixture of Na and powdered WO₃. Since the prepared samples are unstable under the normal conditions, after the shock-wave pressure treatment, the extracted samples were vacuum-encapsulated into quartz ampoules. The ampoules with the samples were stored in liquid nitrogen between the measurements, thus preventing the samples thermal degradation for infinitely long time. Comparison of the ac magnetic susceptibility measured at different magnetic fields and frequencies infers that the superconductivity arises in the metastable weakly linked interfacial regions incorporated into the non-superconducting matrix, which is consisting of the mixture of WO₃, Na₂WO₄, Na₂W₂O₇ and metallic W phases, formed during the shock-wave pressure treatment.

Defect induced metastability and power universality of condensed matter responses on intensive loading

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Defects kinetics is analyzed as specific type of the criticality in out-of-equilibrium system “condensed matter with defects”—the structural-scaling transition. Theoretical and experimental study is devoted to mechanisms of structural relaxation caused by different types of metastable states in condensed matter with defects, strain instability and fracture in a wide range of load intensities. It is shown that the “decomposition” of the metastable states is accompanied by the origin and development of multi-scale collective modes of mesodeflects ensembles (microshears, microcracks) described by the kinetics of two structural variables—defect density tensor having a sense of deformation due to defects, and structural scaling parameter. Defect induced mechanisms of structural relaxation are linked to the generation of different types of the collective modes of defects, that have the nature of self-similar solutions: auto-solitary waves providing the multiscale plastic strain localization and blow-up dissipative structures providing the damage localization kinetics. Dynamics of excitation and evolution of collective modes are linked to the mechanisms of instability and failure in condensed matter with defects and used to explain the original experiments: elastic-plastic transition in shock waves (relaxation of the elastic precursor, universality of plastic wave fronts in metals and liquids), resonant excitation of multiple spall failure and failure waves, spatial-temporal universality of fragmentation statistics in glass and ceramics in wide range of load intensity.

Prediction of the fracture of metals during static and dynamic loading based on the theory of critical distances

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Development of the method for assessing the strength of engineering structures, considering the effects of the non-locality fracture in the area of stress concentrators, under different loading regime is one of the major scientific interests. The theory of critical distances (TCD) is one of the most promising approaches to the prediction of material fracture, in which the stress concentration effect is taken into account. The fundamental idea of the TCD was first proposed by Peterson [1] and further developed by such authors as Novozhilov [2], Whitney, and Nuismer [3]. It was also proved that the TCD can be used to predict the static strength of the notched brittle and quasi-brittle material [4] as well as of ductile metallic material under uniaxial and multiaxial static loading. The idea of the TCD to use one characteristic material length parameter, so-called critical distance L , and linear-elastic analyzes to predict both brittle fracture and fatigue strength. This work presents a design methodology suitable for estimating lifetime under conditions of static and dynamic tensile loading on the cylindrical un-notched specimens and specimens with stress concentrators.

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Research into strength characteristics of fine-grained uranium samples under shock-wave loading

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In addition to earlier published results how quasi-static extrusion of unalloyed technical-purity uranium and its lean molybdenum alloy influences strength characteristics under the quasi-static and explosive loading [1–4]. The paper describes the experimental setup and results of the first 6 explosion experiments where strength characteristics of samples were studied. The samples were manufactured of high-purity fine-grained uranium and uranium that was microalloyed with carbon C and silicon Si. They were shock loaded with AlMn liner 0.5 and 1 mm thick. The multi-channel laser-heterodyne diagnostics was used to record time-dependent velocity profiles $W(x, t)$ and time-dependent displacements $S(x, t)$ at examined portions of the free surface on the samples. Just as in the technical-purity metal and its lean molybdenum alloy, quasi-static extrusion, accompanied by grain refinement and strength characteristics improvements under low-rate deformation, was not observed to seriously manifest itself under high-intensity shock-wave loading.

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Investigation into dynamic deformation of copper and its alloys using composite Hopkinson bars

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The problem of strength and fracture under single loading (such as shock, explosion etc) is particular importance in terms of materials and structures dynamic loading problem. High deformation or loading rates, high stress levels, big plastic deformations as a result of mostly adiabatic deformation process, and specific material response under such loading make it a challenging task to provide background for the development of matter deformation and fracture math models used for the purposes of structural elements properties calculation. Reliability and comparability of the investigation results primarily depend on scientific justification of high-velocity experiments setup. The method of composite Hopkinson bars (CHB), also known as Kolsky method, is one of the methods, having clear theoretical background, high efficiency, flexibility, and reliability of the results. This method allows us to study dynamic stress-strain diagrams at deformations rates $E = 10^2\text{--}10^4 \text{ s}^{-1}$. In the work, we present the results of the experiments where we dynamically compressed copper and copper–tin alloy using CHB method. We determined Dynamic compression diagrams. We also determined Johnson–Cook parameters for copper and copper alloy, this from is widely used in dynamic calculations.

Failure and phase transitions in solid ceramics under uniaxial shock compression

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Ceramics materials attract considerable attention due to their outstanding mechanical properties. Being lightweight, they are also very hard and strong at compression. Thus, ceramics are good for light armors and as an abrasive. However, various experiments [1,2] demonstrate that ceramics strength reduces under shock compression as a result of failure. In this work, SPH-simulations of plate impact experiments [1,2] with silicon carbide (SiC) and aluminum nitride (AlN) are performed. To simulate ceramics failure the improved Johnson–Holmquist–Beissel model [3] is used which was developed earlier for boron carbide (B₄C) simulations [4]. In contrast to B₄C, SiC and AlN undergo a phase transition at pressures 95–105 and 20 GPa respectively, both of which are included in equations of state. Simulation demonstrates good agreement with experimental data. Main features that are representative for shock response of materials undergoing phase transition are reproduced with high accuracy.

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Simulation of mechanical behavior ZrB₂-based ultra-high-temperature ceramics under shock loading in a wide temperature range

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High temperature ceramic materials can be used to create protective and heat-protective structures in hypersonic aircraft, missiles and space landers. The ZrB₂-B₄C composites, have more long term resistant to oxidation than the monolithic ZrB₂ and the melting point above 3500 K, good electrical conductivity. Mechanical behavior of ultra-high temperature ceramics at elevated and high temperatures under shock wave loadings is of interest in connection with the prediction of high-velocity impacts of compact bodies on protective structures. This paper reports results on the investigation of mechanical response of nanostructured ZrB₂-B₄C composites at shock wave loadings in temperature range from 297 to 2000 K. 3D computer simulation of deformation and failure of structured volume of ZrB₂ porous ceramics and ZrB₂-B₄C composites was performed using the multiscale approach. It was shown that dynamic failure of ZrB₂-B₄C nanocomposite has quasi-brittle character in temperature range from 295 to 1473 K. The brittle to ductile fracture transition in ZrB₂-B₄C depends on strain rates. The dynamic strength for ZrB₂ ceramics rapidly decreases at the temperature of 1773 K or above. The rate of growth of the damage parameter at mesoscale level depends on the stress triaxiality. It is shown that the normalized strength at compression of ZrB₂ ceramics and composites ZrB₂-B₄C on the logarithm of normalized strain rate can be described by a power law in the range of strain rates from 10⁻³ to 10⁶ s⁻¹ and temperature range from 295 to 1473 K.

Modeling-based determination of effective mechanical properties of metal–ceramic composites under shock wave loading

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In recent decades, metal-ceramic composite materials are widely used in various fields of industry. This composite materials are often used under extreme operating conditions. In order to evaluate mechanical behaviour of these composites not only experimental methods but also the methods of numerical simulation are widely used. In this paper, the numerical simulation of the mechanical behavior of metal-ceramic composites at the mesoscopic scale level under loading by plane shock waves was made. Also the effective elastic and strength properties of composites with different structure parameters were investigated. Composite material consists of the metal matrix and reinforcing ceramic inclusions. Inclusions have different shapes (arbitrary shape, spherical shape, and shape of short fibers) and are randomly distributed in the matrix. The numerical simulation is performed on a rectangular fragment of the plane section of the plate along the direction of the shock wave front. The mechanical behaviour of the composite is described using the physical and mathematical model of the two-phase condensed heterogeneous medium with an explicit description of its structure. The values of the effective mechanical characteristics of investigated materials were obtained, and the character of the dependence of the effective elastic and strength properties on the structure of composites was determined. The simulation results show that values of effective mechanical characteristics weakly depend on the shape of reinforcing inclusions and mainly are defined by their volume concentration.

Mathematical modeling of the glass-composite reinforcement behavior in concrete under dynamic loading

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The interaction of the glass-composite rod with concrete under the action of an axial tensile load is studied. This task is important in the design of high-rise buildings and structures, and in constructing in seismically hazardous areas. At present, glass-composite reinforcement is widely distributed in residential and industrial construction, but the question of the contact interaction of nonmetallic reinforcing bars with concrete remains poorly studied. An armature rod buried in a concrete sample of 70 mm is considered, that is a special case of application of this element in the energy-efficient three-layered enclosing structures. The rod has a conical extension at the end portion. In experimental studies, the load was created on pile driver by means of impulsive action on the developed stand intended for determination of the anchoring strength of the glass composite rebar in concrete. In a numerical experiment, the problem was solved in a complete three-dimensional formulation. On the interaction interface of concrete and reinforcement, the slip condition without friction was realized. The initial and boundary conditions corresponded to experimental. Comparison of the results of numerical and experimental studies showed a good quantitative and qualitative agreement.

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Modeling of contact boundary destruction at impact interaction of solid bodies

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When developing numerical algorithms and mathematical models that describe the behavior of materials and structures under high-speed interaction, the correctness of the description of the contact interaction plays an important role. When using the Lagrangian approach, in such problems there is a strong distortion of the computational grid, which leads to the inability to perform a calculation. Various approaches to the modeling of the destruction of contact surfaces in the high-velocity interaction of solids in finite element modeling are considered. An algorithm is proposed for calculating contact fracture ensuring the fulfillment of conservation laws. Other approaches are analyzed and comparisons are made with the experimental results.

The work has been conducted with the financial support by grant from the President of the Russian Federation (No. MK-413.2017.1).

Smooth-particle-hydrodynamic mesomodeling of shock-produced ejecta from a randomly bulked layer of spherical particles

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High-pressure shock wave propagation through a layer of bulked spherical particles is followed by formation of dust cloud consisting of fragments of various sizes and velocities [1]. Emergence of such cloud is explained by cumulation phenomenon which takes place because of the collision of neighbor spherical particles accelerated by a shock wave [2].

Previously [2] we presented direct simulation results which revealed the physical processes which take place during the shock propagation. In this work we complete the study by investigating shock propagation in truly random pack structure of particle layer. The newly obtained results are in excellent agreement with the previously presented ones. We demonstrate complex ejecta structure formed in the cloud where transversal velocities play important role in formation of particles inside the cloud. Velocities distribution we obtain is in a good agreement with experimental data [1].

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CSPH&VD³: The massive-parallel load balancing code for smooth-particle-hydrodynamic modeling of materials in extremes

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Application of well-known parallel algorithms for Lagrangian methods like SPH based on static computational area decomposition leads to weak computational resources balance as the algorithms ignore spatial medium redistribution in problems with free surfaces, continuity losses, and high energy density media flows. To overcome the limitation we developed a high-effective parallel program complex CSPH&VD³ (Voronoi dynamical domain decomposition), which uses dynamic decomposition of modeled samples among computational units (CU) according to distribution of the Voronoi diagram cells built upon the samples [1].

Modeling example of a problem with significant surface shape dynamics and highly inhomogeneous spatial density distribution shows a highly effective resources utilization comparing to static domain decomposition. Tests are provided which prove convergence of VD³ algorithm for systems with initial load imbalance with number of particles up to 10^8 distributed among up to 10^3 CU. Almost perfect linear scalability of VD³ is demonstrated.

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Numerical simulation of the propagation of elastoplastic waves in transtropic materials

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At present, the main method for studying the propagation of elastoplastic waves in materials characterized by transtropic elastic, plastic and strength properties is the full-scale experiment. In this case, various mathematical models used in processing the results can be used. In the proposed work, numerical analysis was used to analyze the propagation of elastoplastic waves in transtropic materials using 2 mathematical models: within the framework of the hypotheses of volume isotropy and volumetric anisotropy of deformation processes. Numerical modeling of shock loading of obstacles from transtropic materials was carried out by the finite element method in a three-dimensional formulation. The results of numerical simulation using both mathematical models are compared with the experimental data on the shock load in the directions $[0001]$ and $[101\bar{0}]$.

Mathematical modeling of shock wave interaction with moving and colliding bodies

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The work is devoted to the mathematical modeling of shock wave propagation in the areas with moving bodies. The problem relates to the clarification of the mechanisms of shock wave–particles cloud interaction. Mathematical model is based on two-dimensional Euler equations. The numerical algorithm of Cartesian grid method extends the ideas from [1]. The developed algorithm was verified on a number of test cases about the motion of bodies under the action of pressure force from [1–3]. The detailed simulations of shock wave–one movable cylinder interaction are carried out with classification of possible regimes of flows and wave patterns depending on mass of the cylinder and the intensity of the shock wave. The detailed simulations of the interaction of shock wave with two movable cylinders that can collide with momentum losses are carried out with classification of possible regimes of flows and wave patterns depending on parameters of the problem.

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Mathematical modeling of the instability development on the contact surface of two media under the high-speed impact

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The goal of the work is the qualitative and quantitative simulation of the main features of the natural experiment [1] on the high-speed impact of two metal plates namely the formation of crater-shaped splashes on the surface of one of the plates. Consider the interaction of the lead plate which is thrown with the speed 500 m/s with the steel one. Mathematical model is based on three-dimensional Euler equations for the medium with two-term equation of state. The numerical algorithm is based on Godunov method [2]. Parameters of two-term equation of state were calibrated in [3] using experimental data to get reasonable characteristics of shock waves that are formed after the impact. The special boundary conditions are developed to provide the formation of rarefaction waves that moves into the computational domain after the shock waves reach the free metal surfaces. At some moment after the formation of shock waves the small disturbance of the medium density is applied on the contact surface between the plates. The crater-shaped structure on the contact surface after the passing of rarefaction waves is obtained.

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The shock convergence problem in Euler and Lagrangian coordinates

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The analytical solution of the problem of converging shock and dynamic gas compression was represented in this paper in the following statement. At the initial time a cold gas velocity is zero, and at the external border of the gas set the negative velocity. In other words, Velocity discontinuity is set. After breakdown of a discontinuity the shock will spread from this point into the symmetry center. The boundary moves under the particular law which conforms to the movement of the shock. It moves in Euler coordinates, but the boundary trajectory is a vertical line in Lagrangian coordinates. Generally speaking, all the trajectories of the particles in Lagrangian coordinates are vertical lines. The value of entropy which appeared on the shock retains along each of this lines. Equations that determine the structure of the gas flow between the shock front and the boundary as a function of time and the Euler or Lagrangian coordinate are obtained, as well as the dependence of the entropy on the shock velocity. The problem was solved using original method which differs from the generally accepted ones for constructing self-similar solution. The solution in Euler coordinates was constructed for spherical symmetry [1], in Lagrangian coordinates—for three cases of symmetry: planar, cylindrical and spherical [2]. An algorithm of self-similarity index search was developed. The self-similar coefficients identical to self-similar coefficients from paper [3] were found for a wide range of adiabatic index.

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Two-dimensional computations of optimal solutions of shock wave interactions

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The problems of high-speed collision of bodies and interaction of oblique shock waves incident on the boundary of contact with a substance of higher impedance are considered. In the first case the shape (S) of the colliding bodies is calculated. In the second case calculated S is the boundary of contact of two media. We denote in the first case, T the intersection point of the free boundaries of the bodies, i.e., the point where begins the boundary of contact of two bodies. In the second case, T is the point at which the front of the incident shock wave reaches the boundary of contact of two media. In both cases, the calculated S is such that the speed T is exactly equal to the speed of the shock wave in the substance behind T. Simultaneously with the calculation of S we get solutions of the considered problems. The problem of high-speed impact is a generalization of the problem of high-speed impact of bodies of the same material reported at the previous conference.

Plasticity nucleation in vanadium nanocrystal under mechanical loading

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The investigation of the atomic mechanisms of the plastic deformation nucleation in vanadium crystallites with grain boundaries under mechanical loading was carried out. The simulated crystallite had the form of a parallelepiped and contained a symmetrical tilt grain boundary. The sample was uniformly stretched in the direction perpendicular to the boundary plane. Various combinations of free and periodic boundary conditions were used along the other two directions. The initial temperature of the crystallite was 300 K. Interatomic interactions were described on the base of the embedded atom method. Used potentials allowed describing with high accuracy many mechanical and physical properties which are very important for the simulations of nanoparticle collisions with high velocities. The regularities of local structural transformations in the lattice leading to the nucleation of plasticity in a vanadium crystallite with grain boundaries under uniform stretching were studied. The character of collective atomic displacements causing grain boundaries displacement in bcc materials under high-speed shear loading was studied.

The study was performed within the frame of the Program of fundamental scientific research of National academies of sciences for 2013–2020.

Numerical simulation of cavitating fluid

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Underwater explosions (UNDEX) refer to the detonation of explosive devices immersed in water. Furthermore, in the case of the explosion occurring close to the structure, a high velocity water jet penetrating the gas bubble occurs. This water jet is extremely efficient in producing damage. New experimental data on UNDEX with detailed diagnostics is available recently. Modern CFD tools with new highly efficient numerical schemes applicable for UNDEX simulations were developed and implemented in commercial and open-source software. OpenFOAM is the leading free, open source software for computational fluid dynamics with many different numerical solvers, turbulent, transport and thermophysical models included. UNDEX simulations with OpenFOAM and comparison of numerical results with experiment are shown.

The impact of local current density increase on conductor destruction

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The impact of a pulsed current on materials with micro inhomogeneity of type of crack leads to the formation of a region with increased energy release and heating near the crack top. With a sufficient current density, metal melting in such region leads to crack healing. Due to the reduction in the stress concentration, the strength of the materials increases. However, in the generation of strong pulsed magnetic fields, the same mechanism is one of the limits for the resource of single-turn solenoids, and is manifested in the so-called “saw effect”.

The impact of the pulsed current on materials with defects of type of cracks, which are located in the direction normal to the current streamlines, was experimentally investigated, using the a flat bronze busbar (width—25 mm, thickness—0.25 mm) with cuts of different lengths, loaded with a pulsed current of density 4×10^{10} A/mm² with an effective duration of 3.5–8 μ s, as a sample. After the current has flown near the top of the defect, a circular zone free of material and a growing into the interior of the conductor defect (secondary defect) of type of a crack is observed.

Analysis of the simulation results carried out in the Comsol Multiphysics 5.3A in a three-dimensional formulation has shown that the size of the circular zone free of material, which arose near the top of the defect, correlates with the size of the region in which the current action integral reaches the critical value for the material under study. At the top of the defect, magnetic fields with an induction amplitude of 30–50 T are generated, in which the fracture mode caused by the hydrodynamic flow of the material is typical.

The simulation was carried out at the supercomputer center “Polytechnic” with heterogeneous cluster HPC Tornado.

Non-destructive coils and field shapers for high magnetic field industrial application

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High magnetic field pulse, despite its proven advantages, has still not been widely adopted in industrial application-mainly because the critical parameter of work-coil service life.

PULSAR research and development works aimed to create suitable work-coils (solenoids) for industrial use are reported here. The material and geometry considerations are addressed.

One-turn coils with or without power-pulse transformers were designed, manufactured and tested at a wide range of both dimensions and work regimens, including water cooling and air cooling systems. A contact system for the coil out at peak current of about 1 MA has been developed and tested too. Magnetic field distribution has been checked as well, and water cool solenoid tested to 50 000 pulses life time at 25 T and 4 pulse/min.

Compact magnetic cumulative generator with fast open switch

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Magnetic cumulative generators (MCG) with an inductive load up to 1 μH were studied in experiments. A fast explosive open switch was used to shut off an electric current in a primary circuit. The MCG operation and the switch run were synchronized. Divergent cylindrical detonation in the switch was attained by special lay-out of elastic explosive. The efficiency of MCG with the open switch was estimated and compared with conventional MCG efficiency. Operation of the MCG was described in the frames of multi-circuit model with time-dependent parameters. The recorded current derivatives and the shape of voltage drop on the load were close to simulated values.

Generation of microwave radiation at detonation of condensed explosives

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Wide-band microwave radiation ($f = 0.1\text{--}10$ GHz) was registered at explosions of condensed HE charges of weight up to 10 kg. The radiation intensity surpassed intensity of thermal radiation. An attempt to explain this phenomenon has been carried out. The suggested mechanism consists in following: during expansion of products of detonation a highly non-equilibrium medium is generated, oscillatory temperature of which can essentially exceed rotational one. Such environment is basically active from the point of view of generation and amplification of microwave radiation. As an air behind a shock wave is strongly ionized, the radiation can leave the explosion zone boundaries only after the decrease of this ionization. HE detonation generated the microwave radiation at the time moments corresponded to estimated moments.

Preparing and some properties of spheroid epsilon hexanitrohexaazaisowurtzitane

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In this work, based on the experience of obtaining spherical crystals of trinitrotriazacyclohexane (RDX) and tetranitrotetrazocane (HMX) by spheroidization (intensive mixing of slurry in a special vessel), spherical crystals of hexanitrohexaazaisowurtzitane (HNIW) from two types of crystals were obtained. The crystals of the first type were obtained by evaporation crystallization and had bipyramidal shape. The crystals of the second type were obtained with use of modifying agent and had a round shape. The density of obtained spherical crystals of HNIW was determined. Infrared spectroscopy was used to confirm the polymorph and the absence of inclusions and modifying agent in the crystal structure. As a result of experiments on spherical crystals of HNIW was shown that the original morphology of crystals influences the final morphology of the crystals subjected to the process of spheroidization. The measured sensitivity of different morphology of HNIW to shock and friction showed that the lowest sensitivity to friction have crystals obtained during spheroidization.

Detonation properties of hydrazine nitrate

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The use of hydrazine nitrate (HN) $N_2H_4HNO_3$ as one of components of rocket fuels requires determination of detonation parameters, sensitivity to shock wave impact, the critical conditions of detonation of this explosive. Experimental investigation of these values is an aim of this work. The results of the experiments show that the detonation properties of HN have a number of features that are not typical for pressed high explosives. First of all, it should be noted the low shock-wave sensitivity, which is much lower than that of TNT. For the samples with the density 1.68 g/cc an appreciable chemical reaction rate behind the front of initiating shock waves is observed only at pressures above 20 GPa. High detonation velocity $D = 8.92$ km/s was recorded for steady-state detonation wave in the charges HN with initial density 1.68 g/cc. The change in the detonation velocity with the variation of initial density is not monotonic, but has a characteristic s-shaped form: in the density range 1.5–1.6 g/cc, D increases sharply with increasing density. We can assume that the detonation regime is unstable in the neighborhood of initial density 1.55 g/cc and minor differences in the structure of charges, conditions of initiation and other factors that lead either to attenuation of the detonation, or the transition to detonation branch corresponding to an ideal detonation.

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

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In 1981–1983, L V Altshuler and G S Doronin with their colleagues observed the mode of undercompressed (weak) detonation in phlegmatized explosive compositions. A specific feature of this mode is the self-similar expanding region of the steady-state flow behind the near-front peak of the pressure and mass velocity. The focus of this effort is studying mode details. The VISAR technique and the laser-heterodyne technique (PDV technique) was used to study the plasticized RDX. The explosive composition—lithium fluoride (LiF) interface velocity was recorded at the time by exit of the plane detonation wave. Initiating system has included the explosive lens, TNT–RDX booster ($60 \times 10 \text{ mm}^2$), and the 5-mm thick copper base-plate. We recorded time profiles having a near-front peak and a plateau with the follow-on dip.

Testing the assemblies for impact loading of a flat recovery ampoules with a continuous pressure hold

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The shock compression of powder materials is used for the synthesis of new materials or phase states [1]. For these purposes are often used the flat ampoules with the studied material inside. To implement a pressure the impact scheme with flat liner is applied [2]. Due to the small liner thickness, the loading time of the material inside the ampoule does not exceed a few microseconds. In some cases, such duration of loading is insufficient to complete a synthesis to a new phase state. This paper describes the probation of schemes for loading the recovery ampoules during longer time. As the test object under loading a synthesis of a cubic structure (γ -phase) of silicon nitride (Si_3N_4) from the original hexagonal structure was chosen. Previously this process was carried out in mixtures of Si_3N_4 with bromide [3] and potassium chloride, and with copper powder, at pressures up to 50 GPa [4]. In addition, it was carried out under filling the initial pores in silicon nitride with liquid bromoform (CHBr_3) [1]. Shock loading was carried out in counter and reflected shock waves, time of loading was evaluated by $x-t$ diagram and the pressure—by the known shock adiabats of the assembly elements. The effective duration of loading depended on the size, strength and mass of assembly elements. The x-ray analysis were carried out on diffractometer DRON-2, $\text{CuK}\alpha$ radiation.

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Initiation of reaction in powder mixtures Al–CuO under different rates of thermal load

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In the publications, there is a considerable variation in the measured speed value of the combustion of the metal oxides–metals mechanically activated powder mixtures [1]. Therefore, there is no definite interpretation of the reaction propagation mechanism. Largely the variation may be due to the mixtures preparation and different conditions of initiation, behavior and measurement of the combustion process. It is believed that for combustion of such mixtures there is no “initial conditions memory effect”. Only the current settings are significant: the mixture density, particle size, dose of mechanical activation. However, in this study we investigated the role of conditions of the reaction initiation. For initiating the reaction in a stoichiometric mixture of Al–CuO powders (bulk density 2.2 g/cm³) we used a thin nichrome wire heated by a constant power current or the electric charge (1 μ s) in the short spark gap (1 mm). The fact of ignition was fixed by the signals of the photodiode, electric contact sensor and pressure sensor. The heating energy of the wire was determined by power source and by signals from sensors. The ballast resistance in the discharge circuit of the capacitor changed the value of the current in the spark. The reaction develops through the appearing of reactive (excited) particles at discrete points of contact during a short “induction” time. Then the ignition starts into a volume of primary energy dissipation. The data for estimating ignition energy and for determining the dependence between the duration of the “induction” period and the source power were obtained.

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Combustion dynamics of Al–CuO powder mixtures in a square channel with a transverse magnetic field

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Earlier [1] we have investigated the combustion dynamics of the Al and CuO powders mixture in the conditions of natural or stimulated scattering of products. Irrespective of a way of initiation of reaction, the combustion area is characterized as a stream consisted of the cold and reacting components surrounded by the radiating plasma of reaction products. However, the last measurements have shown incomplete spatial correlation of areas of radiation and conductivity. In the report the results of a research of combustion dynamics of similar mixture in the square channel with a section of $10 \times 10 \text{ mm}^2$ and 100 mm long are given. Micron-sized powders of initial components were mixed in a stoichiometric proportion and subjected to mechanical activation. The sample weighing 1 g (bulk density) was placed at the closed end of channel. Initiation of chemical reaction was carried out by a plasma of electric charge with a power contribution 1 J during $1 \mu\text{s}$. The chemical energy release generated a stream of mixture components and continued behind a cut of the channel. Outside of the channel around median section were placed neodymium magnets. The cross-section potential in the flow was recorded on a six thin parallel wires. Besides, in two sections of the channel outside of magnetic field was placed two wire electrodes with the set potential. On a cut of the channel was placed a lightweight piezoelectric sensor, and at some distance from a cut—the photo diode. The light emission from scattering hot products was fixed by a high-speed camera.

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Studying of the combustion mechanism of nanothermite composites

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Thermite is a combustible mixture of metal and oxide of a less active metal. In case of nanoscale components the properties of the thermite mixtures are significantly changes. The deflagration speed in some cases is up to 2 km/s. In thin channels is observed stable propagation of combustion waves, sensitivity to friction and electrostatic discharge increases. The significant change in these characteristics is usually associated with a qualitative change in the combustion mechanism for nanothermites. The significant changing of these characteristics is usually believed to be linked with a qualitative changing in the combustion mechanism for nanothermites. However, at the present time there is no unified opinion on the combustion mechanism of nanothermite mixtures. In this paper, we present the results of the experiments on the determination of the combustion waves parameters for the CuO/Al nanothermite mixture are recovered by the dynamic x-ray method by means of the synchrotron radiation. This work was supported by the Russian Foundation for Basic Research (grant No.17-33-50202).

Effect of aluminum on the detonation characteristics of emulsion explosives

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The emulsion explosive (EMX) is one of the most general industrial explosive. Aluminum powder in the amount of up to 15% by weight is often used in the EMX. The addition of aluminum increases the power of the explosive composition, and also affects on its sensitivity and stability. In spite of the wide application of the aluminized EMX, the effect of aluminum on the detonation characteristics of EMX has not been completely investigated. In the article [1], the pressure and temperature profiles for EMX with various aluminum contents were obtained. On the base of the analysis of these profiles the authors concluded that aluminum reacts behind the Chapman–Jouguet plane. In this paper, our experimental data are compared with those known from the literature. Comparison of the pressure, temperature and electrical conductivity profiles allows us to predict the reaction path of detonation products with aluminum which differs from proposed in [1].

[1] Lefrancois A, Grouffal J V, Bouinot P and Mencacci S 2002 *Proc., Symp. Detonation* 432–9

Explosion of aluminized mixtures in the bubble column as a method of underwater blast wave enhancement

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As previous experiments with small aluminum-rich charges exploded in small-scale water volumes have shown, excess aluminum quite efficiently and fast reacts with surrounding water increasing the overall specific explosion energy to values that are much greater than those underwater high explosives. Small-scale experiments demonstrated that the mechanical impact of explosion of such energetic materials can be locally enhanced several-fold by generating in water bubble arrays. The aforesaid findings call for checking in larger-scale tests with the use of appropriate instrumentation. The results of experiments of underwater explosions of ideally and nonideally detonating charges in continuous water and in water containing freely ascending air bubbles are reported. Charges weighing ≈ 10 g were exploded in a metal reservoir filled with water. Parameters of compression waves were measured with pressure gauges. Mechanical impact of explosions was assessed with an accelerometer mounted on a movable target. Factors influencing formation of directed compression waves after explosion in water containing air bubbles are ascertained. The results obtained made it possible to formulate the conditions under which nonideally detonating energetic materials explode with high energy efficiency and enhanced mechanical impact, they include optimal compositions of the mixture, mutual positions of a charge and target, parameters of a bubble array in water etc.

Detonation synthesis of non-agglomerated metallic nanoparticles deposited on carbon supports

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Synthesis of nanoparticles is carried out by thermal decomposition of organometallic complex compounds in the detonation front of explosives, where the temperature reaches several thousand degrees. The low concentration of metals in the total mass of the charge leads to the formation of single non-agglomerated nanoparticles deposited on detonation carbon. At the same time, the morphology of detonation carbon and its amount depends on the properties of the explosive. The metallic nanoparticles in detonation products are determined by the high-resolution transmission microscopy. Depending on the conditions, the rounded particles with sizes from 1 to 100 nm are formed. The formation of nanoparticles behind the detonation front is observed by the dynamical measurements of small-angle x-ray scattering of synchrotron radiation during the detonation. This work was supported by the Russian Foundation for Basic Research (grant No. 16-29-01050).

The dynamics of carbon nanoparticles size at the detonation of TNT–RDX charges

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During the detonation of oxygen-deficient high-explosive nano-sized condensed carbon particles are formed. At that, the time of particles forming depends on the charge diameter.

In this work, we carry out the dynamic measurement of small-angle x-ray scattering (SAXS) during the detonation of molten charges of TNT–RDX of 20, 30, 40 mm in diameter. The dynamics of the average size of carbon particles are recovered from the SAXS data. Scattering centers with an average size of about 4–6 nm are formed at the time less than the resolution of the technique (0.5 μ s behind the detonation front). After that, we observe their growth during several microseconds. The time of nanoparticle growth behind the chemical reaction zone increased from 3 to 6–8 μ s when the charge diameter was enlarged from 20 to 40 mm.

The work is supported by the Russian Foundation for Basic Research (project No. 16-29-01050).

Thermal stability of detonation nanodiamonds at elevated temperatures

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The physical dates for explosive of detonation nanodiamonds (DND) demonstrate significantly contradictions in the literature. Literature analysis showed that the boundary of thermal stability of DNDs is the solid phase transition of diamond sp^3 phase to graphite-like sp^2 phase. The method of synchronous thermal analysis was used for determination of parameters of thermal stability of detonation nanodiamonds. The experiments were carried out at temperatures range from 30 to 1500 °C at atmospheric pressure in dynamic argon environment. Heating rates were 2 and 10 °C/min. After heat treatment the saved samples were investigated by the x-ray, Raman spectroscopy and scanning electron microscopic.

In the results our work, influence of as temperature and well as the rate heating was found on the powder parameters. In our experimental conditions, the decreasing of diamond phase starts significantly above 600 °C in the sample [1]. But the thermal stability some diamond nanoparticles are above 1500 °C [1]. Influence of the heating treatment rate affects on sizes of powder nanoparticles conglomerates. In particular the formation of layer structure was observed after heat treatment with rate 2 °C/min up to 1500 °C in the sample.

The thermal stability value is extremely important for hardening of steel details surface. Obtained results of nanodiamonds thermal stability allowed us to recommend the temperature for making of target from chromium–nanodiamond mixture, which was used as media for steel details surface coating.

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Main physical processes of fracture propagation in silica-based optical fibers under intense laser irradiation

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Propagation of a laser-induced damage in transparent dielectrics is complex physical event. This event depends on variety of parameters (laser intensity, pulse length, photon energy and band-gap value). Physical processes from initiation (loss of transparency) to material destruction depend on energy deposition dynamics and dielectric properties. Prominent role among transparent dielectrics belongs to silicon dioxide. In particular, silica is one of the main working media for powerful optical fiber lasers. Silica-based optical fiber is convenient target for studying the solid density plasma interaction with cold silica.

Such conditions are realized in optical fiber at laser-driven detonation [1]. Used laser let us obtain damage trek near hundred own core diameters during one laser pulse. Besides, the using as target the core of silica-based optical fiber has some diagnostic advantages. It allows supply the same form of energy deposition in every cross section of optical fiber. Tested regime demonstrates near constant velocities during 250 ns in the range of laser intensity 2–4.5 GW/cm². The formation of cracks and the rate of laser plasma expansion determine the front of absorption velocity. Possible models of phenomenon are discussed.

This work was carried out due to support by basic research program of the Presidium Russian Academy of Science No. I.31P.

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A theory of detonation-like waves of spin reversal in molecular magnets

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Molecular magnets are crystals of metal-organic compounds in which molecules have a substantial magnetic moment (e.g. manganese-12 acetate, Mn_{12}). The crystal magnetization in an external field directed along its easy axis is maximal. Importantly, however, there can be an asymmetry that makes one of these directions energetically preferable. That is, one of the states of maximal magnetization is metastable, while the other is stable. Transition from the metastable to stable state can occur either homogeneously throughout the sample or in a wave-like manner. In the latter case, one possibility is a deflagration-like wave that is controlled by heat conduction. Another possibility is a supersonic detonation-like wave, which was observed experimentally and was analyzed theoretically in [1] assuming a steady ZND-like structure with Arrhenius kinetics and non-ideal equation of state (EOS). Here we extend the theory of [1] to include time dependence and derive a reduced model that shows that the ZND-like waves can undergo instability depending on the magnitude of the external magnetic field and the crystal initial temperature. The instability manifests itself in periodic or aperiodic pulsations of the wave strikingly similar to those of pulsating detonations in gases [2]. Furthermore, we show that the reduced model is almost identical to the toy model of detonations that was proposed in [3].

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[3] Kasimov A R, Faria L M and Rosales R R 2017 Theory of supersonic waves of spin reversal in molecular magnets

Mathematical modeling of detonation initiation and propagation in the complex-shaped domains

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The work is devoted to the development of the numerical algorithm for the mathematical modeling of gaseous detonation initiation and propagation and the complex-shaped domains using fully unstructured computational grids and high-order numerical schemes. Mathematical model is based on two-dimensional Euler equations supplemented with the one-stage chemical kinetics model. Numerical algorithm is based on the finite volume approach, advection upstream splitting method (AUSM) numerical flux and the reconstruction of the grid-functions on unstructured grids [1]. The canonical problem of cellular detonation formation is considered as the test case. The influence of grid resolution and the properties of the numerical scheme on the results of modeling is investigated. The problem of the critical geometrical conditions determination for the detonation initiation and propagation in the asymmetrical tube with variable cross section area filled with stoichiometric hydrogen–air mixture is considered. The problem in consideration relates to the utilization of the industrial waste [2].

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Multiscale smoothed-particle hydrodynamics and molecular dynamics simulation of detonation

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Detonation initiation phenomenon [1] in condensed matter requires development of multiscale simulation techniques. Contact smoothed particle hydrodynamics [2] is natural for mesoscopic simulation of complex geometry and tracking the media behind shock front. Reactive molecular dynamics in a model of explosive is employed to calibrate chemical decomposition mechanisms and equation of state. An isochoric thermal decomposition time is determined within achievable region in molecular dynamics. In consistent hydrodynamic simulation of detonation a deduced kinetic scheme is implemented. This kinetic scheme defines transition of reagents to products if an isochoric thermal decomposition time, corresponded to the current state of smoothed particle, is lesser than one hydrodynamic step.

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[2] Medin S A and Parshikov A N 2010 *Teplofiz. Vys. Temp.* **46** 973–980

Study of effects of nano-additives on combustion and detonation of the energetic materials

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Performance of the energetic materials (EM) can be enhanced significantly with the addition of nano-additives. When the additives are in the nano size range, they offer unique advantages which can eventually enhance performance of the EM. In this paper, we present the results of usage of artificial neural networks (ANN) technologies, for the creation of new kinds of computational models of the EM combustion and detonation that can solve difficult experimental tasks in combustion research speedily and easily. In this connection, the first multifactor computational models of the combustion and detonation of the EM with such nano additives as metals, metal oxides, metal salts, metal composite materials, organ metallic compounds, termites and carbon nanomaterials will be presented. The results obtained depict that ANN technologies could be considered as a good approximation tool of the experimental functions of several variables, a good tool for the generalization of the connection between variables of combustion experiments, an instant engineering calculator specializing in combustion tasks, a useful learning tool for studying combustion behaviors, an affordable way to receive “new” experimental results, and a good tool to present experimental results for scientific community.

Combustion of foamed emulsions containing biochar microparticles: Foam as a medium for incomplete oxidation of hydrocarbons

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The work is devoted to experimental study of the process of combustion of foamed emulsion containing biochar particles. Combustible foamed emulsion represents a brand new type of combustible system that can be used to solve the problems related with incomplete oxidation of hydrocarbons.

Foamed emulsion is a multiphase system consisting of oxygen bubbles dispersed in the emulsion. The emulsion represents a water solution of stabilizer with heptane drops distributed in it. Biochar microparticles were added into the prepared emulsion in the concentration from 0 to 35 g/l. Despite the volumetric water content in the initial emulsion was 82.4% the flame propagation in such foam was possible. On the other hand the high water content favors the realization of suitable conditions for incomplete hydrocarbon oxidation (the quenching of intermediate oxidation products takes place). During the experimental research we analyzed the combustion products composition with the use of chromatograph. It was obtained that the dependence of hydrogen, carbon monoxide, acetylene and methane contents on the biochar particles concentration is characterized by a certain minimum. Experimental results show that the foamed emulsion can serve as a perspective medium for synthesis of valuable components for chemical technology and energy production from renewable bio-resources.

The work was funded by grant from the Russian Science Foundation No. 17-19-01392.

Excitation of acoustic oscillations arising from combustion of coal dust in the channel of variable cross-section

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Theoretical study of excitation of acoustic oscillations arising from combustion of coal dust in the combustion chamber of a pulsed Magnetohydrodynamic generator was carried out. The combustion chamber is a cylindrical pipe of variable cross-section. The flow in the combustion chamber is considered one-dimensional. Mixing in the longitudinal direction is absent. It is considered that the particles of coal dust are monodisperse and have a spherical shape. It is believed that the combustion of the coal particles occurs in the diffusion mode. The heat capacity C_p is assumed constant. The Lewis number is assumed to be equal to unity. The damping force acting on the coal particles during their motion in an acoustic wave was determined according to the Stokes law. In this paper, it is shown that acoustic oscillations decay in an expanding channel, but intensify in a narrowing ones. In the paper, formulas for calculating the frequency and the increment of acoustic oscillations are obtained.

The structure of the flow behind the shock wave in a channel with a comblike structure of obstacles

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The propagation of a pressure wave in a channel with periodically located obstacles is numerically investigated. It is shown that in such a channel there can be a discontinuity with the structure. The structure of the discontinuity is the leading shock wave and relaxation zone. The change in the flow parameters within the structure is close to periodic with time. The distribution of the gas parameters within the structure over space has the character of damped oscillations. The pressure pulsations are caused by waves that circulate in the space between the obstacles, reflecting from the upper and lower walls of the channel. Flow parameters behind the structure remain practically constant and do not depend on time, although the velocity of the leading shock wave periodically depends on time. An approximate relation is obtained that relates the parameters of the gas behind the structure of the discontinuity with the average structure velocity. Calculations of the average velocity of the structure, velocity, and density of the gas behind the structure from a given pressure are in satisfactory agreement with the gas-dynamic calculation data. It is shown that in the case of periodically located rectangular obstacles, the parameters behind the structure of the discontinuity depend on the channel geometry, including height, obstacle width and distance between them only through the parameter α , which is the ratio of the volume of the area between obstacles to the volume of the area above obstacles. The approximate dependences obtained allow us to make an estimate of the minimum pressure at which a current with a discontinuity structure exists. This estimate is confirmed by gas-dynamic calculations.

Interaction of spherical shock waves with a heterogeneous layer with a chemically active gas phase

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In connection with the great difficulties in the experimental study of the destruction of moving bodies, great importance is attached to methods of mathematical modeling of processes that determine the behavior of cosmic bodies in the atmosphere, and it becomes necessary to study the effect of the energy of chemical reactions initiated by a shock wave on the interaction of a shock wave with a plane surface. When entering the dense layers of the atmosphere, a space body drastically loses its speed. The resulting pressure in the shock layer can measure up to thousands of atmospheres; significant radiant heat flows and inertia forces are generated. Due to high stresses inside the body, its complete or partial destruction occurs, accompanied by the release of energy. The interaction of the radiant energy with the trees leads to the release of gaseous products of pyrolysis and ignition [1, 2].

In this paper, a model problem is solved on the interaction of spherical shock waves with a heterogeneous layer near a plane surface [3]. The heterogeneous layer is a two-phase medium consisting of solid particles and a chemically active gas phase. It is shown that the oxidation reaction leads to an accelerated rise in temperature and pressure in the gaseous phase and promotes an increase in the propagation velocity of the shock wave in a heterogeneous medium.

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Development of the key experimental approaches for investigation of shock wave front in gases

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In our early work [1], we had reported about non-equilibrium emission in shock wave front in noble gas with a small addition of heavy molecules. Now the structure of the shock wave front has been studied by new experimental techniques for noble gas with a small addition of heavy molecules. The distribution density near the shock wave front is measured by a modified laser schlieren method. The spatial resolution of this method is commensurate with the free path length in paired collisions of heavy particles. The found experimental techniques had been realized on a high-vacuum shock tube. The residual pressure of background gas in experiments did not exceed 0.01% of the concentration of a small additive of heavy molecules. The developed approach allowed to detect the phenomenon not observed earlier: sporadic radiation of hot spots in the front of uv propagating in a mixture of noble gases. The work was supported by program of the Presidium RAS No. 13 “Condensed matter and plasma at high energy densities”.

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Emission of CH* and C₂* during the high-temperature oxidation of propane in reflected shock waves

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The autoignition of a stoichiometric propane–oxygen mixture diluted with argon was studied behind reflected shock waves in the temperature range of 1230–1700 K at the total concentration of $[M]_{50} \sim 10^{-5}$ mol/cm³. Emission signals from electronically excited CH* (at $\lambda = 429$ nm) and C₂* (at $\lambda = 516$ nm) radicals were recorded. It was found that the CH* and C₂* emission time profiles reached their maxima almost simultaneously over the entire temperature range covered. The temperature dependence of the ignition delay time measured from the time of reaching the maximum by the CH* emission signal was simulated within the framework of several published data kinetic mechanisms. It was found that, at temperatures below 1400 K, all the kinetic models tested predict ignition delay times several-fold longer than that experimentally observed. Using a sensitivity analysis to the reaction rate constants in the induction period, the main reactions that affect the ignition delay time were identified.

Experimental studies and detailed kinetic simulation of the influence of acetone and propane additives on soot formation in the reflected shock waves

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Experimental studies and detailed kinetic simulations of the formation of soot particles during pyrolysis of mixtures of acetylene with acetone and propane behind reflected shock were carried out. The acetone and propane additives substantially promote the process of soot formation as compared with acetylene-argon mixtures. Detailed kinetic simulations closely reproduce our own experimental data. The kinetic model of soot formation was comprised of 4782 direct and reverse reactions involving 372 species. The predictive possibilities of the kinetic model of soot formation were tested for the case where acetone and propane additives were added to acetylene-argon mixtures. Note that all the kinetic parameters of the unified kinetic model were kept constant. That the indicated additives enhance the soot yield were interpreted based on the results of kinetic simulations, more specifically, the process in acetylene-argon mixture proceeds only through a single polyynene-dominated pathway of soot nucleation, while addition of acetone or propane opens an additional aromatic pathway of soot nucleation, thereby increasing the overall soot yield.

Application of ARAS method for ethanol with oxygen reaction study behind shock waves

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The most of published reaction-rate constants of interaction between biofuels and oxygen are measured in the low-temperature region (300–500 K). Using these constants for real combustion temperatures is possible only by extrapolating them to the high-temperature range, which leads to significant errors. As a result, the temperature range under which the actual combustion of biofuels takes place remains poorly understood. The direct measurements of the reactions rate constants between biofuels and oxygen in a high-temperature (900–1500 K) range is an urgent task. Reliable data in this temperature range can be obtained in a shock-tube experiment using the precise measurements of small atomic concentrations by the method of atomic resonance absorption spectroscopy (ARAS) in the vacuum ultraviolet. The appearance and consumption of oxygen atoms during the reaction of ethanol and oxygen at 900–1300 K and 2–3 bar behind reflected shock waves using ARAS measurements on resonant oxygen atom line at 130.5 nm have been carried out. As sources of oxygen atoms for reaction with ethanol nitrous oxide was used, dissociation of which into an oxygen atom and a nitrogen molecule is considerable already above 900 K, when the thermal dissociation of ethanol does not yet begin. The temperature dependence of the rate constant of the reaction of ethanol with oxygen was obtained. The data are analyzed and compared with the results of kinetic modeling using the Chemkin package. The work is supported by the Russian Foundation for Basic Research (grant No. 17-08-01303).

The experimental study of C_3F_7I dissociation kinetics using atomic and molecular resonance absorption spectroscopy methods

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Currently, halogenated hydrocarbons are widely used in various industries for increasing explosion safety. However, the need to protect the ozone layer of the Earth's atmosphere has pushed to search for new, efficient and at the same time environmentally friendly fire extinguishing substance. Among the most promising additives, iodine-containing halogenated hydrocarbons, including C_3F_7I , are of increasing interest. The molecules of C_3F_7I are completely ozone-friendly and non-toxic for humans. Nevertheless, for industrial application, it is first necessary to investigate in detail the kinetics of dissociation of both C_3F_7I and its secondary components. Reaction $C_3F_7I + Ar$ reaction was studied by sequential application of atomic and molecular resonance absorption spectroscopy using resonance line I at 183.04 nm and CF_2 radical band at 251.9 nm behind reflected shock waves. The experiments were performed at the temperatures from 900 to 1500 K and pressures of 2.5 to 16 bar. The initial concentration of C_3F_7I in Ar varied from 1 to 500 ppm. The time profiles of CF_2 and I concentration, forming at C_3F_7I dissociation were obtained. From these experimental data the temperature dependences of the rate constants of CF_2 and I formation and their activation energy were determined. This fact allowed to study in detail the kinetic mechanism of C_3F_7I decomposition in a wide range of temperatures. This work has been supported by grant from the Russian Science Foundation No. 14-19-00025P.

The study of CF_3I thermal dissociation kinetics using atomic resonance absorption spectroscopy method behind shock waves

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Experimental studies have been carried out on the application of the highly sensitive method of atomic resonance absorption spectroscopy to measure the time profiles of iodine concentration at a wavelength of 183.04 nm produced by pyrolysis of the CF_3I combustion inhibitor. The experiments were performed behind reflected shock waves at temperatures of 900–1250 K and a pressure of 2–3 bar. The rate constant of the dissociation reaction of CF_3I was measured at low and high pressures. The obtained values of the rate constant are compared with the known literature data. The data obtained in the course of the complex study provide new valuable information on the activation energies and rates of the most important reactions, which are not yet available in the world literature. The use of these data makes it possible to carry out a detailed analysis of the mechanisms of action of the test inhibitory additives on combustible mixtures. This work has been supported by grant from the Russian Science Foundation No. 14-19-00025P.

On the impossibility of suppressing of methane ignition by the additives of halogenated fire suppressants

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An influence of the additives of iodine-bearing halogenated fire suppressants CF_3I and $\text{C}_3\text{F}_7\text{I}$ on shock-induced ignition of methane–oxygen mixture $6.7\%\text{CH}_4 + 13.3\%\text{O}_2 + \text{Ar}$ at pressures 4.0–6.5 bar was studied experimentally. Observed temperature dependencies of induction times have shown that these suppressants, while being effective as inhibitors of hydrogen ignition [1], contrary reduce the ignition delay time in methane similarly to other halogenated compounds studied previously [2].

Performed kinetic analysis indicated that considered fire suppressants are incapable of inhibition of methane autoignition at elevated temperatures due to release of active radical, initiating chain combustion reactions. It is shown that hypothetical suppressant with desired inhibition properties should remain more stable at high temperatures and, at the same time, have more chemically active molecule. Such requirements seem to be rather contradictory.

Suggested simplified model of suppressants promotion and inhibiting proves that that more than ten-fold increase of the radicals consuming efficiency would be required to at least compensate promotion effect, and furthermore to noticeably slow down the ignition. Obtained results allowed to conclude that effective chemical inhibition of shock-induced methane autoignition by the halogenated hydrocarbons is unlikely.

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On the effect of oxygen additives on the formation of a detonation wave in acetylene

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Acetylene is an exothermic hydrocarbon compound. At pyrolysis of acetylene a graphitized soot and molecular hydrogen with release of 227 kJ/mol are formed. The self-decomposition of acetylene can proceed as in a combustion mode, with the speeds from 10 to 50 cm/s, and in a detonation mode with speeds more than 2000 m/s [1,2]. These properties of acetylene could be used for environmentally friendly power installation, producing energy without exhaust of carbon dioxide. However an important problem has to be solved—how the parameters of the detonation wave of condensation are correlated with the convenient detonation wave?

In this work a detailed experimental and numerical analysis of the interrelation between thermodynamic and kinetic processes during the condensation and oxidation of acetylene and its influence on the development of detonation is carried out. A mechanism of the transformation of the detonation wave of condensation in acetylene into convenient detonation wave with oxygen addition is developed. The results of the experiments and numerical simulation showed that the characteristic times of acetylene oxidation in the traditional detonation wave are much shorter than the characteristic times of formation of soot particles in the detonation wave of condensation. The obtained results can be used to develop optimal operating regimes for new environmentally friendly energy devices based on the use of thermal and kinetic energy released in the detonation wave formed during the condensation of a strongly supersaturated carbon vapor.

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The influence of methane and hydrogen on the temperature changes during pyrolysis of acetylene in a heated gas flow

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Investigation of initial stage of formation of carbon nanoparticles in the gas phase is essentially important and necessary task. The purpose of this work is the experimental study of the initial stage of the process of carbon nanoparticles growth in a pyrolysis flow reactor at atmospheric pressure. Experiments were performed in the flows containing 30% C₂H₂, 30% C₂H₂ + 45% CH₄ and 30% C₂H₂ + 7.3% H₂ diluted in N₂. Infrared temperature measurements in the wavelength range 1.86–2.16 μm were carried out in different flame conditions and flame heights (varied between $H = 20$ –100 mm above the burner) and also in radial position. Two types of conically tubes were applied to protect the flames: (a) a tube with $l = 45$ mm and (b) a tube with $l = 7.5$ mm. These tubes were positioned directly above the sinter plate of the burner. The experimental data on the radial temperature measurement were processed using the Abel transformation to obtain a temperature profile along the radius in the flow at different heights. This study was supported by the Joint Project of German Research Foundation and Russian Foundation for Basic Research No. SCHU-1369/24-1 and No. RFBR-16-58-12014.

Role of methyl radicals in soot formation

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Soot formation is an important both in terms of reduction of harmful combustion emissions and synthesis of nanomaterials. Possible way to control the soot formation process is the injection of chemically active additives to the combustible mixtures. Experimental study of methyl radical influence on soot formation during acetylene pyrolysis behind shock waves was carried out. The experiments were carried out in standard shock tube reactor. The laser light extinction was used for soot volume fraction measurements and laser-induced incandescence was used for carbon nanoparticles sizing. Acetylene is a key intermediate specie in soot formation in combustion and pyrolysis of hydrocarbons. Methane, dimethyl ether (DME) and diacetyl were used as additives to the acetylene. Methyl radical is a main product of first decomposition reactions of methane, dimethyl ether and diacetyl. The fivefold increase in soot volume fraction with addition of 1% of methane to 2% of acetylene diluted in argon was observed. The less significant increase of soot volume fraction with addition of diacetyl was observed. And negligible increase of soot volume fraction with addition of DME was observed. Moreover, the additions of methane and DME caused the soot formation at less temperatures comparing to pure acetylene mixtures. The kinetic modeling for investigated mixtures was carried out. The probable kinetic mechanisms of methyl radical influence are discussed. This work was supported by the Joint Project of the German Research Foundation grant No. SCHU-1369/24-1 and the Russian Foundation for Basic Research grant No. RFBR-16-58-12014.

Experimental study of the role of excited radicals in inhibition of hydrogen–oxygen mixtures ignition

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The goal of this study was the experimental investigation of the emission spectrum in the uv and ir region of electronically and vibrationally nonequilibrium radicals and molecules, their effect on the ignition of hydrogen and the search for inhibitors and promoters for control the process of ignition. The ignition was registered with a pressure sensor, as well as by the emission of OH at 310 nm. The observed temperature dependences of the ignition delay are in agreement with the literature data and results of numerical kinetic simulations. One of most important radical in hydrogen–oxygen combustion is hydroperoxyl HO₂ [1]. It was experimentally found that the ir emission from the radical HO₂ is fully screened by the strong emission of H₂O which is the main product of combustion. In the uv region nonequilibrium radiation was detected at the wavelength of 220 nm corresponding to electronically excited radicals HO₂ and H₂O₂ presumably. The observed signal shape was similar to the radiation signal of OH radicals. The experiments with small addition of potential relaxant or inhibitor (CO₂, C₂F₄Br₂, CCl₄) were carried out. It was found that almost all additives result in a significant increase of radiation. The kinetic calculations based on assumption of equilibrium in degrees of freedom of species have shown that for correct description of observed experimental dependencies by the concentration time profiles of the radicals the literature kinetic mechanisms have to be complemented with the elements of non-equilibrium kinetics.

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Suppression of detonation in hydrogen–air mixtures

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The dynamics of the detonation wave in gases, its intensity and decay into the shock wave and the flame front substantially depend on the presence of acoustic-absorbing elements. The main reasons for the suppression of detonation, apparently, are the disappearance of transverse waves, heat loss in a porous medium, and flame stretching [1]. The purpose of this paper was to study the dynamics of the flame front and shock wave in a porous channel by means of schlieren photography, to determine the dynamics of a porous material and the effect of this dynamics on the detonation decay process in mixtures of hydrogen with air. The decay of the detonation and the propagation of the flame in the hydrogen–air mixture were experimentally investigated in a detonation tube of rectangular cross-section with solid walls and two types of porous coatings. Two types of porous coatings were used: polyurethane foam with 95% porosity and steel wool with a porosity of 99% and an average fiber size of 0.03 mm. The decay of the detonation wave into a shock wave and the flame front was studied with the help of a shadow device IAB-451 and a spark source with pulse duration of 1 μ s. The dynamics of the front of the flame was recorded with the help of a high-speed camera “VideoSprint” with a frame rate of up to 200 000 frames per second. Shadow shots of the decay of a detonation wave into a shock wave and a flame front are presented. The decomposition was observed when using both the polyurethane foam and the steel wool. It was found that the distance between the shock wave and the flame front increases as the wave moves along the porous section of the detonation tube.

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Lean spherical hydrogen–air flames at 4 orders of magnitude in size and energy

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Free spherical premixed flames propagation is studying in volumes of cubic centimeters to hundreds of cubic meters. Ignition energies range from parts of a millijoule to tens of kilojoules. Typically, the authors compare the results with similar scale data. Experimental studies of flame propagation in a wide range of scales are not available in scientific literature. The subjects of the present work are identification of features of common and different for the flame propagation in volumes from 4 liters to 40 cubic meters; comparison of the flame propagation modes upon ignition with energies from 1 mJ to 5 J; explanation of differences in results when using different shells that limit the volume of the combustible mixture. A series of experiments on spherical propagation of flame front in various shells is conducted. The position and morphology of the flame front was recorded with infrared camera Infratec ImageIR 8320 with spectral range 2–5.7 μm and schlieren device IAB-451 equipped with high-speed camera Videosprint G2. Dependences of the flame front position versus time are obtained.

The study is supported by the Russian Science Foundation (grant No. 14-50-00124). Large scale experiments were conducted using the equipment of the Moscow Regional Explosive Center for Collective Use RAS.

On the structure and stability of ultra-lean flames

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The hazards related to gaseous explosions demand the accurate estimations of the stable combustion limits. Moreover, it is of paramount importance to obtain a detailed pattern of all the possible combustion regimes developing in near-limit combustible mixtures. Present work studies the peculiarities of combustion in ultra-lean hydrogen–air mixtures. On the basis of numerical analysis, it is shown that the ultra-lean flame can exist in the form of stable flameball in terrestrial gravity conditions. Herewith, the buoyancy force affects greatly the flameball structure via the heat and mass transfer driven by the formed convective flows. At the final stages of its evolution, the flameball propagates upwardly with almost constant terminal speed, while a set of independent satellite flame kernels detached from the main flame core propagates in the thermal wake behind the flameball determining the effective growth of the flame. It should be also noted that due to the peculiarities of flameball structure the temperature of combustion products is superadiabatic. Therefore such a flameball could easily induce ignition in the upper layers of the stratified hydrogen–air atmosphere where more reactive gas containing a larger amount of hydrogen is located due to natural convection.

Expanding hydrogen–air flames over the heat absorbing substrate

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Free spherical premixed flames propagation is studied for a long time and up to now there no agreement between different descriptions of experimental data. The subject of our investigation is slow hemispherical flame front propagation over heat-absorbing substrate in a quiescent premixed hydrogen–air at constant pressure.

A series of experiments on hemispherical propagation of flame front is conducted. In one part of the experiments the surface was a continuous flat aluminum plate. In another part of experiments aluminum plate was covered with 50 mm layer of steel wool. The position of the flame front was recorded with infrared camera Infratec ImageIR 8320 with spectral range 2–5.7 μm . Dependences of the flame front position versus time are obtained. Measurements the position of the flame front show the front slowdown at the propagation of a flame front over the heat absorbing substrate. Calculation of heat absorption in the steel wool layer shows that the heat losses due to the absorption are sufficient to reduce the flame front speed, which is observed in the experiments. The use of heat-absorbing coating is promising as a passive safety system which reduces the flame speed and shock loads caused by the gas explosions.

The study was performed under grant from the Russian Science Foundation No. 14-50-00124.

Numerical simulation of air–hydrogen mixture detonation burning in exhaust manifold of model high-altitude test facility

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Test facilities for perspective high-speed air engines with simulation of high-altitude flight conditions are equipped by explosion-proof system for the case of unburned air–fuel mixture penetration and ignition in exhaust manifold. Safety valves of this system are intended for pressure reduction when deflagration burning. The aim of this work is estimation of maximum pressure level at manifold walls and safety valves efficiency when detonation burning. At first, the process of homogeneous air–hydrogen mixture slow burning to detonation transition near the tube wall was analyzed. For this purpose by means of the software complex developed in Central Institute of Aviation Motors and been based on Godunov's finite difference scheme of increased accuracy order the two-dimensional unsteady tasks of flame propagation with account of chemical reactions kinetics were being solved. The principal differences of this process passage in tubes of different diameter are showed. The task of detonation wave propagation in bended duct was being solved in a flat formulation. The possibility of geometry scaling for more detail resolution of complicated structures arising in the process of detonation wave interaction with the wall is demonstrated. The calculations made it possible to estimate the maximum pressure. In all calculations it exceeded 10 bar at initial pressure of the mixture 0.2 bar. Moreover, gas outflow through the safety valves was no influence on detonation wave intensity.

Working process research of gas-piston engine on hydrogen fuel

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The diesel engine is being upgraded in the laboratory of Joint Institute for High Temperatures Russian Academy of Sciences. The aim of this work is the change in structural units and measuring systems installed under another type of fuel—hydrogen and synthesis gas. This work will explore a number of important problems, advantages and benefits of energy production with alternative renewable fuels. This subject is of great importance for the future of humanity, as it will to some extent cease to be strongly dependent on exciting reserves of mineral resources—oil and gas.

Flow patterns near the micron particle surface in the process of gas ignition

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An important role in ignition and combustion of gaseous mixtures belongs to the non-uniformities of the flow related with reactor geometry and some impurities of the mixture. This work studies the ignition event taking place near the micron particle in the flow of compressed gas behind the shock wave. Since it is quite complicated to study the ignition of gaseous mixture seeded with particles (because of its intransparency), the research is based on the numerical approach. On the basis of numerical analysis the structures of the flow and temperature fields in the vicinity of particle surface are demonstrated. It is shown that there are two possible ignition regions: at the frontal surface of the particle and in the wake behind the particle. Flow deceleration and its multidimensional development determines the local formation of hot regions (hot spots) playing the role of ignition kernels. Due to the fact that the particles distributed in the gas flow could become ignition kernels the limits of shock-induced ignition can become significantly wider in comparison with pure combustiblegaseous mixture. As a result the measured ignition delays can be much shorter compare with predicted values for examined mixture. Parametric study of the described phenomenon by means of numerical analysis allowed us to obtain certain data on ignition delay shortening for hydrogen-oxygen mixture of different compositions at different initial pressures.

Control of dynamic stall in a wide range of Mach numbers by nanosecond surface dielectric barrier discharge plasma actuators

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High speed helicopters must accommodate significant changes in the rotor lift performance as a function of rotor angle. The advancing blade can achieve transonic conditions while the retreating blade experiences relatively low speed. The high Mach number of the advancing blade requires an angle of attack below 5 degrees for maximum lift, whereas the retreating blade requires high an angle of attack in excess of 10 degrees. Under high speed and high load conditions, stall occurs during the retreating cycle and destabilizes the aircraft. Thus operation requires that the angle of attack of the blades be changed during the cycle and optimized with flight speed. The focus of this research is to determine to what degree plasma actuators can be used to optimize high speed flight performance, particularly focusing on suppressing the dynamic stall by retreating blade separation control.

Experimental study of coupled acoustic and electric discharge effect on methane–air flame

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The development of advanced power-generating plants based on high-speed combustion chambers requires the solution of a number of fundamental problems. In particular, the important task is the flammability limit expansion in the high-speed flows. As one of the cleanest fuels methane becomes more and more popular in new designed engines. A new method of coupled acoustic and electrical discharge treatment of premix combustion of methane–air mixture was studied. Experimental data of blow-off limits of a laminar and turbulent flame under the wide flow-rate range are presented. The effect of the acoustic waves and high-voltage electric discharge on blow-off limits, velocity fluctuations and flame characteristics is shown. Under the experiments exciting acoustic frequency was varied in the range 10–1000 Hz with amplitudes up to 140 dB. It is shown that acoustic and electrical discharge treatment can provide changes in stabilization conditions and intensification of laminar and turbulent combustion under the wide ranges of mixture equivalence ratio and flow Reynolds number.

The study was performed under a grant from the Russian Science Foundation No. 17-79-10503.

On the modeling of free and channel shear turbulent flows via CABARET numerical method

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In this paper we present the results of modeling of laminar and turbulent Taylor-Green vortex decay, which is one of the canonical problems of computational hydrodynamics. The system of Navier-Stokes equations was solved on a sequence of refined grids with 64^3 , 128^3 , 256^3 cells at Reynolds numbers $Re = 100, 280, 1600, 4000$. The main properties of the numerical method are discussed on the basis of an analysis of the kinetic energy dissipation rate and integral enstrophy curves, time evolution patterns of spanwise vorticity, energy spectra, and spatial correlation functions.

The second part of the paper deals with the turbulence generation, which is specified on an unstable velocity profile of a thermally viscous fluid in a nonisothermal temperature field. The problem was solved in a three-dimensional domain with various boundary conditions (non-slip, periodic and quasiperiodic with constant pressure gradient along the length of the channel) posed on the boundaries. We treat the flow basing a global averaging of the turbulent characteristics involved in the equation for turbulent kinetic energy, i.e. an advection, a pressure diffusion, a turbulent transport due to triple correlations, a molecular dissipation, a production, and a turbulent dissipation.

Unsteadiness of shock wave boundary layer interaction

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Interaction between shock wave and boundary layer can cause boundary layer separation. Turbulent boundary layer separation is non-stationary phenomenon [1]. Influence of wall temperature condition on the separation region unsteadiness was investigated. Separation of turbulent boundary layer was studied in supersonic flow on the compression ramp with angles of 23° and 30°. Wall temperature condition was described by temperature ratio T_w/T_∞ and was altered in range of 1.6–3.11. During the experiments averaged velocity and root-mean-square (RMS) velocity fields of separation region were obtained by means of Partical Image Velocimetry. Averaged velocity fields was used to measure reattached boundary layer thickness and velocity profile. For adiabatic wall reattached boundary layer has thickness about 4.2 mm and 6 mm for 23° and 30° ramp, respectively. For heated wall condition boundary layer thickness increases in both cases. Comparative analysis of separation on 23° and 30° ramp has shown that for equal separation length reattached boundary layer thickness has almost the same value. RMS velocity fields have shown regions of velocity perturbation. According to the experiments most perturbed area is at the separation position. Reattachment region also has strong perturbation. These regions of velocity perturbation are related to the separation boundaries oscillation. For both 23° and 30° ramp Increasing temperature ratio causes prolongation of perturbed regions. Length of these regions mainly depends on temperature ratio and and weakly depends on separation length.

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Study of wave dynamic impact of an underwater burst on a submersible

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Gas and oil rigs to be served by manned and unmanned submersibles are one of the promising hydrocarbon production technique in the Arctic shelf. To meet an ecological safety requirement different emergency situations must be accounted for. The wave dynamic impact of an underwater burst (when ice sheet is to be broken with explosives) is one of the emergency situations. The paper provides a methodology developed for math simulation of the wave dynamic impact of underwater bursts of any nature upon submersibles that takes into account the medium two-phase state. The methodology takes into account geometry of a submersible and a rig, variations of the submersible position relative to sand-bed and the rig, evolution of gas cavities in liquid medium, compressibility of the liquid medium. A series of simulation cases corresponding to operation conditions close to real were run. Different hydrodynamic patterns of flow around the submersible as well as gas cavities of different configurations were considered. Pressure on the surface of the submersible and the rig was taken as a criteria to evaluate the effect of different varying parameters. Impact of an underwater burst was estimated for different operation conditions, different distances from a submersible to a rig and different spacial position of the burst epicenter. A grouped burst impact, including the asynchronicity of bursts, was estimated. The wave dynamic impact on stability of the submersible motion was also considered. Requirements to configuration of protective gas cavities to reduce dynamic impact on the submersible and rig were set.

Investigation of hypersonic conic flows generated by magnetoplasma light-gas gun equipped with Laval nozzle

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A new method of hypersonic flows generation is proposed, and the results of an experimental study of hypersonic flow over cones with half-angles of $\tau_1 = 3^\circ$ and $\tau_2 = 12^\circ$ are presented in this work. The Mach numbers of studied incident flows were $M_1 = 18$ and $M_2 = 14.4$, respectively. The use of a light-gas gun [1], where an accelerating channel was replaced with Laval nozzle, allows to obtain a hypersonic outflow with optical density sufficiently high for flow visualization and diagnostics with the help of optical methods. The flow structure was visualized by means of Schlieren method with use of straight Foucault knife [2]. Shadowgraphs were recorded by high-speed camera with frame rate of 300 000 fps and an exposure time of 1 μ s. The Mach number for the incident flow was calculated from the inclination angle of the shock wave on shadowgraphs.

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Basic features of high performance code for computation of hypersonic flows

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Recently, computational model has been developed to numerically simulate three-dimensional hypersonic flows. The model has been realized as high-performance (HPC) code. The code can solve hypersonic flows around bodies of arbitrary shape considering conjugate heat and mass transfer on the surface, surface deformation due to ablation process. Most recently, the computational model has been updated to enhance overall performance. New code realizes a coupled solution of three-dimensional unsteady Navier–Stokes flows and heat problem in the interior of the body. Heterogeneous mesh topology can be used both in the flow region and in the wall one. Heterogeneous computer architecture (central or graphic processing unit—CPU or GPU) is utilized. Fast and robust grid reforming procedure was implemented. The key update is new fully implicit method for calculating hypersonic flows using multi-GPU architecture. The performance of the new code is demonstrated on calculation of $M = 30$ flow around a sphere using 850000 grid cells. Older explicit solver on one GPU has shown to be 50 times faster than one-core CPU version. New solver enhances the performance of explicit one by 7–12 times.

Numerical study of combustion wave propagation initiated by discharge

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To provide a high efficiency and low toxic emission operation of internal combustion engines, low temperature combustion strategies have been considered in the last decade. Usage a homogenous charge compression ignition (HCCI) engine is considered more effective than the spark engine. Nevertheless it is hard to ignite lean mixtures (fuel–air equivalence ratio < 1) with compression only and one need to find some ways to initiate combustion. It is common knowledge that preliminary discharge treatment of the fuel–oxidizer mixture may significantly reduce the induction time of the ignition [1]. Previous research [2] shows that discharge treatment mainly affects combustion due to appearance of chemically active particles. In this work two steps of ignition are simulated: discharge activation of mixture and following evolution of combustion. Concentrations of chemically active radicals and temperature rise after discharge stage are initial parameters for continuous-fluid-dynamics modeling of combustion. Authors carry out 1D numerical simulation in cylindrical coordinate system and show that discharge activation allows to ignite lean mixture with initial condition corresponding to HCCI operating cycle ($T = 600\text{--}900\text{ K}$, $P = 6\text{--}40\text{ atm}$). It was found that time for combustion wave formation and for autoignition of total volume depends on specific energy and size of the discharge area. The specific mechanism of ignition acceleration due to discharge treatment is discussed.

This work was supported by LIA KaPPA–RFBR grants No. 17-53-16003 and 17-53-16002 (France–Russia).

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Determination of the helical vortex cross section shape moving stationary in the cylindrical tube

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The shape of the helical vortex moving stationary in the cylindrical tube is analytically found in this work. Inside the core, a uniform vorticity distribution is assumed. To solve the problem the algorithm proposed by Norbury (1973) was used. The shape of the vortex core is found from the integral equation for the stream lines enclosed the core. The problem is reduced to finding the Fourier series decomposition coefficient.

Particle shadow velocimetry technique application for two-phase flow study

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This paper is devoted to the droplet size and velocity measurement PSV (particle shadow velocimetry) technique [1] study and application. High-magnification shadow Imaging is very suitable for visualizing particles, droplets and other structures. The technique is based on high resolution imaging with pulsed backlight illumination. This technique is independent of the shape and material (either transparent or opaque) of the particles and allows to investigate a particle size of $7 \mu\text{m}$ [2]. Particle size, velocity, concentration, shape and distribution, mass flux can be obtained using PSV technique. This technique is unique and does not have any analogs in Russia.

The experimental optical scheme adjustment was realized during the work. A series of experimental researches for disperse characteristics determination and visualization of the aerosol formed by the front-line device of low-emission combustor of gas turbine engine were performed for different modes of operation.

The comparison of results obtained by two measurement techniques was carried out. The first technique is well known developed method of phase-Doppler particle analyzer (PDPA) and the second one is a new and unique PSV technique.

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Numerical study of various factors influence on the efficiency of hydrogen combustion in high-speed air flow

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With an increase of the hydrogen–air mixture speed, the rate of change in the concentration of the components due to chemical reactions becomes comparable with the corresponding rates due to convective and diffusion mixing. This leads to the necessity to use the mechanisms of chemical kinetics in the numerical modeling of hydrogen combustion in the air flow. The known combustion mechanisms for a hydrogen–air fuel mixture are considered in the work: Dimitrov, Jachimovsky, Hanson–Hong. Numerical modeling of hydrogen combustion in a high-speed air flow was carried out using the indicated mechanisms. The factors influencing the combustion efficiency are determined and quantified: the length of the channel, the speed of the air flow, the equivalence ratio, the number of struts, the ratio of struts dynamic pressures.

Analysis of development trends of power-units for high-speed flying vehicles

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The review of modern achievements in the field of development of high-speed flying vehicles with a power plant is presented, based on the information available in open sources. Modern development projects for such vehicles are considered. The ways of solving the problems connected with the creation of high-speed aircraft with power plants based on scramjets are analyzed.

Investigation of thermal condition of model channel of a complex shape at the supersonic flow of a multicomponent radiating and reacting gas mixture

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In the present paper, the problem of determining the thermal state of a complex shape channel under the flow of a high-speed reacting flow in it is considered. A reliable determination of the flow path walls thermal state becomes possible when solving the coupled heat transfer problem. As the object of investigation, a channel of variable cross-section was chosen. Outside, the channel is cooled by hydrogen in a supercritical state. The walls of the channel on the outer side are smooth. The study is mainly aimed at determining the proportion of radiant heat flow, its effect on the overall thermal state under different flow regimes in the channel, including thermal locking. The problem was considered in a two-dimensional formulation for different values of the mass flow of hydrogen. In this case, a complete Favre averaged system of Navier–Stokes equations for nonstationary turbulent reacting flows was solved with closure using the one-parameter model of Spalart–Almaras turbulence. The thermophysical properties of hydrogen in the supercritical state were described using polynomial dependencies.

Experimental-calculation study of the heating and cooling process of the discontinuous type cowper heater with ball inserts

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A device is needed to ensure its heating up to sufficiently high temperatures for testing with the use of high-enthalpy air flow. An important role plays the chemical composition of the air flow, especially when simulating flow parameters close to full-scale heater. The cowper type heater of discontinuous action with ball inserts allows to obtain the total temperature of the air flow over 1800 K, while not distorting the chemical composition of the air. When developing and working with such a heater, the complex physico-chemical processes occurring in the working volume of the cowper heater are taken into account. An actual scientific task is to obtain integral characteristics of cowper heater, as well as its design and layouts. In this paper, a method has been developed for the analytical calculation of non-stationary heat exchange in a cowper heater, which is verified by numerical modeling. The thermal and hydraulic characteristics of a cowper discontinuous type heater can be determined with application of this technique.

Computational research of solid hydrocarbon sublimation in gas generator

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Nowadays gas generator development for producing cold fuel-rich flow, as a result of solid hydrocarbon sublimation, is an important task in the diverse industry fields. The presented work is devoted to computational research of solid hydrocarbons sublimation process under the high-enthalpy gas flow. Mathematical model was developed and validated by known experimental data. On the basis of computational results the criteria of solid hydrocarbons sublimation course was obtained under the impact of turbulent flow. Sublimation products mass flow rate and temperature dependencies from various gas generator operating parameters were estimated.

Numerical and experimental study of heater for liquid and gas fuels

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During ground tests of some power plants, it is necessary to realize the heating of liquid and gas fuels for imitation of operation working regimes. This work contains results of numerical simulation and experimental tests for the heater of cowper type, which is used for liquid and gas working medium. Results of parametrical research of air heating were presented. It was carried out the comparison of calculation results with results, obtained during experiment. As a result of conducted studies it was found good correspondence numerical and experimental results and defined the regularity of heat transfer at heater channel at different working parameters.

Calculation of cryogenic propellant system of high-speed aircraft

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Cryogenic fuels utilization appears to be promising for aircraft engine, namely, condensed natural gas, liquid hydrogen, propane, etc. The urgency of switching to cryogenic fuels is due to their high heat of combustion, cooling capacity, environmental safety, significant natural reserves and low cost. The task of the work is modeling and thermal-hydraulic optimization of the cryogenic fuel system by reference to specific features of its use in the high-speed aircraft and in particular: long endurance, high heat-transfer intensity, variety of operation conditions, alternating G-loading etc. To solve the presented scientific problem, the mathematical model and the parameters calculation procedure of cryogenic fuel system have been developed, which makes it possible to carry out parametric and optimization studies in a wide range of operational conditions. The work presents the results on the selection of cryogenic fuel system parameters for a advanced high-speed aircraft on cryogenic methane. The main mechanisms of the various factors influence on the fuel system mass characteristics and the losses by fuel gasification have been obtained.

Flow simulation around the heat-loaded element under the supersonic test facility conditions

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Experimental research of the heat-loaded model elements is essential part at the early stages of aircraft development. Experimental research is comprised of ground testing of the elements, which prototype the parts of a high-velocity aircraft made of heat-resistant material. The approach flow parameters should correspond to the flight conditions. Temperature of the aircraft parts can attain flow total temperature, and it leads to thermal strain of the most materials at high flight velocities. A thin metal sheet of heat-resistant material was used as the layout of heat-loaded aircraft elements for ground testing. Numerical simulation of the test samples was made for materials resistibility examination. Static pressure and temperature distributions on the samples surfaces in the test stand were obtained under the defined flow conditions. Mach numbers fields and flow streamlines are shown at the symmetry plane of the stand operating region.

The implementation of turbulators for the controlling of the boundary layer

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In this article within the study of the turbulators influence on the working conditions of the air intake, the calculated and experimental results are compared. The calculations of turbulators were made with the help of numerical simulation in a three-dimensional formulation using the example of a single-shot model of the air intake. The experiment was made in a pulsed wind tunnel with a profiled nozzle with Mach number at the outlet $M = 3$. The atmospheric air was used as working gas with a braking temperature of 293 K. The stand model of the single-screw air intake makes it possible to change the height of the throat, so that it is possible to accurately determine the boundaries of the launch of the air intake. The results of the calculation were compared with the experimental data obtained with the help of the Tepler system and pressure sensors placed along the path of the model. The calculations showed that the air intake start with the turbulators occurred at a lower throat height, and as a consequence, with a higher compression ratio of the gas in the flow path. These results were confirmed during the experimental work. Thus, the use of turbulators makes it possible to increase the limits of autostart and the efficiency of the air intake.

Numerical modeling of liquid hydrocarbons combustion using the hybrid Reynolds averaged Navier–Stokes and large eddy simulation turbulence model

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Numerical modeling of liquid hydrocarbons injection and combustion in the air stream with temperature more than 900 K inside constant cross-section extended channels is presented. Various options for spray injector arrangement in space are considered, and effect of excess oxidant ratio variation (from 1 to 2) on combustion process is investigated. The research is performed with Ansys Fluent continuous fluid dynamic numerical simulation software. Combustion law for fuel is described with one quasiglobal reaction. The dependence of reaction rate from temperature and local turbulence parameters is considered. For consideration of turbulent structure features DES (detached eddy simulation) turbulence model is applied. The technique for combustion completeness coefficient estimation for the elongated channel length by means of unsteady data fields averaging is presented. Different types of transition process in the channel after fuel supply are revealed: ignition in trailing torches, ignition and stabilization of a flame in a backflow zone. Experimental study is performed using a model mounted at the on-ground test facility with attached air duct. Comparison of simulation results and experiments has shown satisfactory coincidence of fuel burning-out process integral characteristics.

Numerical simulation of flow in gas-dynamic critical section

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During autonomous adjustment of operation process in combustion chambers of high-enthalpy flow generators, during the tests of high-temperature structural materials, which are used for combustor manufacturing, it is necessary to regulate the constriction degree for combustor outlet section. The purpose of this is varying of velocity and density of flow in combustor duct. Using of evident mechanical way of regulation is conjugated with difficulty of realization of reliable construction and movable part actuator, which can work for a long time in condition of high-temperature flow. Throttling is another way of constriction regulation for outlet combustor section. The main advantages of this way are technical simplicity of realization, absence of movable parts, and smoothness of regulation. The disadvantage of this mean is presence of additional degree of freedom. It appears in non-linear dependence of pressure in combustor from combustion product flow rate at constant feeding of throttling gas. The aim of this work is determination of flow pattern in gas-dynamic critical section at different means and parameters of throttling gas injection. Research was carried out with help of numerical simulation for ideal gas flow. Main varying parameters were geometry of injection area, pressure, temperature and adiabatic coefficient for main air, which was flowing through combustor. On the base of realized calculations it was built the dependence of combustor constriction degree from gas characteristics and pressure ratio for main and throttling gases. The effect of injection way was shown.

Experimental-theoretical method for estimating the parameters of a high-enthalpy flow in channels of constant cross section

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Using techniques, taking into account the features of the organization of the working process in the channels of variable cross-section, the evaluation of the completeness of combustion of hydrocarbon fuel under different conditions of gas-dynamic flow throttling in the channel was made on the basis of the experimental data obtained. The calculated and experimental dependence of the pressure in the channel on the flow rate of the main gas and the air flow on the throttling is determined. Numerical methods, taking into account the thermodynamic composition of the products of combustion of hydrocarbon fuels, sputtering and evaporation, obtained theoretical distributions of the parameters of the high-enthalpy flow (temperature, combustion completeness, pressure, etc) along the channel cross-sections. The difference in the results of determining the completeness of combustion and temperature by numerical methods and according to the results of the experiment was no more than 5.3%.

Methodology of the output airflow momentum determination in channels of variable cross-section

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The flow momentum is an important gas dynamic parameter characterizing the combustion and mixing processes in channels of variable cross-section. Development of procedure based on the recalculation of parameters diagnosed in experiments with the use of a specialized physical and mathematical apparatus is required to determine it during experimental studies of combustion chambers model flow duct of advanced power-generating plants.

The developed algorithm and the results of its approbation with reference to ramjet module of a perspective power plant traction characteristics determination are presented. Calculation and following comparison of the data obtained with the use of the developed algorithm with the results of direct measurement of the force created by the experimental object are carried out. Inaccuracy of calculations is less than 8 percent. On this basis, conclusions about the operability and the possibility of applying the proposed algorithm for determining the output momentum of the airflow in the variable cross-section flow paths are made.

Combustion of boron-contained condensed particles in high-enthalpy airflow experimental-calculation study

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Today the issue of boron-contained condensed particles combustion in high-enthalpy airflow is important for understanding working processes. For creating methods of burning intensification for boron-contained condensed particles in bounded space it is necessary to conduct experimental and calculated research.

The description of model laboratory facility and method of experimental definition of combustion completeness is presented. The method deals with gas and condensed phase gasification products of boron-contained power-consuming condensed composition in high-enthalpy subsonic airflow. The mathematical model of particles combustion, obtained by experimental data, is presented.

The results of complex experiment-calculated research of two-phase fuel mixture combustion process in uniform cross section channel with temperature up to 2500 K, pressure 0.1–1 MPa and excess oxidant ratio 1.5–2 are given. Mechanism of temperature and oxygen ratio influence on the particles combustion rate are detected. Presented data can be useful for experiment-calculated research of working processes in energy-power plant.

Distributed plasma system for ignition and flameholding in supersonic flow

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Previously it was shown that ignition and flameholding of gaseous and liquid hydrocarbon fuel is feasible by means of surface dc discharge without employing mechanical flameholders in a supersonic combustion chamber [1]. However, high power consumption may limit application of this method in a real apparatus. This experimental and computational work explores a distributed plasma system, which allows reducing the total energy consumption and extending the life cycle of the electrode system. The numerical simulation helped to improve a geometrical configuration of the test cell. It was found that the tested electrical scheme with shared ground electrode has some advantages in comparison with non-interacted plasma loops. Also it was shown that distributed plasma system, consisting of two plasma modules, accelerates the combustion process comparing to a single plasma module. These test series, at some extent, verify the two-stage mechanism of plasma-assisted ignition [2]. This research was supported by grant from the President of the Russian Federation No. MK-1734.2017.8.

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Application of spark discharge for mixing in supersonic flow

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Previously it was shown that the spark discharge could be used as an actuator for mixing of gaseous fuel with the supersonic airflow [1]. Later it was shown that curved spark discharge produces a fast jet structures and mechanism of jets formation was discussed [2, 3]. Results of further experimental and numerical investigations of afterspark channel in ambient air and supersonic flow are presented in this study. It was experimentally confirmed using high speed 8 frames camera that each bend of the long spark discharge channel produce a fast jet in ambient air. The inflow of cold gas from the near electrodes space into the center of heated zone of the afterspark hot cavity was observed for long spark. Application for mixing by spark discharge located near wall in the area of CO₂ gaseous jet in supersonic flow was investigated in numerical parametric study. This research was supported by Russian Science Foundation grant No. 17-79-10494

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

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Dielectric (transformer) oils are used in electrical engineering in power and measuring transformers, as well as in oil circuit breakers, in which accidents can occur because of internal short circuit and arc discharge development, which can lead to the destruction of the oil-filled equipment casing. In spite of the fact that in the presence of gas bubbles in a liquid dielectric, a partial discharge can occur in a gas bubble in fields smaller than necessary for oil breakdown [1], interest in recent years to gas-liquid media is associated with their damping properties, which may be sufficient to prevent destruction of the oil-filled equipment casing due to short circuit. The experimental stand was created to study the damping properties of the gas-liquid mixture the classical method of electrical explosion of wire was used. Microbubbles 1 and 0.5 mm in diameter are generated with tangential gas supply in the narrowing part of the Venturi tube [2] and Laskin tube. Experimental allowed to obtain synchronized current-voltage characteristics of the discharge, as well as the dependence of the intensity of finite amplitude waves propagating in the mixture of transformer oil with gas bubbles, on the degree of gassing and the bubble size in the mixture. The intensity of waves of finite amplitude decreases strongly in the gas-liquid medium. The work is partly sponsored by Russian Foundation for Basic Research grant No. 17-08-00110.

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Formation of craters, seas and mascons on the Moon by galactic comets

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The hypothesis [1, 2] is discussed, according to which craters with a diameter $D \geq 10$ km on continents of the Moon, like the continents themselves, as well as sea basins without mascons and with mascons, are formed by bombardments of galactic comets [3]. The last bombing, which mainly determined the modern exterior of the Moon and other planets, took place between 5 and 1 million years ago. At that period ≈ 5 galactic comets could fall on area 100×100 km². At such density of cometary fallings, crater funnels are superimposed, the diameter of the resultant crater increases, its morphology becomes more complicated, and the energy of impact heating of the rocks increases. We believe that the lunar seas being formed by this mechanism. They have a diameter $D \geq 160$ km, and their formation is accompanied by greater heating of rocks and origin of more magmas. Even greater heating and formation of magmas occur in the basins with $D \geq 218 \pm 17$ km [4], where mascons arise [5]. Herewith, if in ordinary craters and seas, melting processes encompass rocks of Moon cortex, in seas with mascons are melted the more deeply lying rocks of lunar mantle.

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A dynamical model as a shock wave pattern to predict the shape of some craters

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The shape of the crater allows estimating or describing what happened from the moment of impact until the crater develops on the surface of the celestial body. Then, it is possible to develop a theoretical dynamic model to predict the formation process of the crater after the fall of the meteorite. In this document, a new shock wave pattern is applied along with a new model for the formation of the crater to predict a typical crater shape. Although we are concentrating on being able to compare these analytical predictions with high resolution images previously taken, these new analytical tools seem to be promising enough to become a good result at the moment.

Methods of interpretation of seismic signals of high-speed impacts to a lunar surface

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The problem aiming qualitative change of an Apophis orbit when its movements in Solar System comes to an end is formulated in [1, 2]. Instead of passive saving tactics the variant of use of this asteroid is considered for realization of large-scale space experiment. This experiment is shock interaction of an asteroid and the Moon.

In the present work methods of interpretation of seismic signals of high-speed impacts to a lunar surface are considered. It is supposed that signals are registered by rare network of seismic stations. The optimizing problem of minimization for divergences (between the values of transit time of P-waves which are experimentally measured and theoretically calculated) is solved for estimates of these parameters.

Methods for determination of parameters of a seismic source are considered. Basic parameters of impact are: time; location (width and longitude) and kinetic energy.

The approaches and methods used for specification of the Moon structure on the basis of the analysis of seismic signals are discussed. Work is made with support of the Russian Foundation for Basic Research project No. 15-08-08615.

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Calculation of parameters of the seismic waves which are formed at high-speed impact by an asteroid Apophis on the Moon surface

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Use of an asteroid Apophis for realization of a large-scale space experiment was offered earlier [1]. Experiment consists in the organization of shock interaction of an asteroid and the Moon. Initiation of large-scale collision will allow to answer a number of the physical questions concerning the Moon. In the present work the 2D-method of calculation of seismic waves propagating in multilayered structure of the Moon is offered. This method is synthesis of a finite-difference method and analytical method of expansion in a series. The problem is considered in the spherical system of coordinates. The solution is expanded in series on the angular coordinate (the latitude of the locality). The system of the differential equations for the series coefficients depending on radial coordinate and time decides by finite-difference method. The structure of the Moon is specified according to speed model by Latem and Toksotsu [2]. Calculated parameters of seismic waves are used for definition of number and the locations of seismic stations. Requirements to the accuracy of measurements of seismic characteristics are formulated. Work is made with support of the Russian Foundation for Basic Research project No. 15-08-08615.

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Molecular dynamic simulation of explosive origin of planets satellites

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The explosion in the planets interior and throw out part of its outer layers onto orbit with the satellite formation helps to explain features of the elemental and isotopic composition of the Moon. Computer simulation of the satellite origin was solved in a 2D setting method of molecular dynamics with the number of particles up to some hundred thousand.

The role of particles played bodies by asteroid size of order 100 km, interacting by the Newton low. Substance properties in condensed state adopted as short distance potential. Some calculations with a variation of initial conditions allowed confirming explosive scenario of the Moon origin and showing its advantages over other hypotheses.

Smart control by micro-scale oscillatory networks for enhanced operational capabilities of the solid propulsion systems

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Spacecraft systems and equipment are extremely sensitive to combustion instabilities which can cause undesirable problems and creates the need for control. Fundamental understanding of the micro-scale combustion mechanisms is essential to the development of the next-generation technologies for extreme control of the propellant thrust and control by combustion instabilities. Both experiments and theory confirm that the micro-scale oscillatory networks excitation in the solid propellants reactionary zones is a rather universal phenomenon. In accordance with our new concept, the micro- and nano-scale structures form both the fractal and self-organized wave patterns in the energetic materials reactionary zones and can be considered as a fingerprints of the set of holograms of the reactionary zone. In particular, for each exact frequency of the oscillatory process in the reactionary zone corresponds the unique self-organized spacial patterns of the micro- and nano-scale. A novel strategy for smart real-time control of the thrust and combustion instabilities in solid propulsion systems are based on control by self-organization of the micro-scale oscillatory networks and self-organized patterns formation in the reactionary zones with use of the system of acoustic and electro-magnetic fields, generated by special kind of the electric discharges along with resonance laser radiation. The electric discharges also are capable for excitation of the wave patterns in the reactionary zones. Application of special kind of the electric discharges demands the minimum expenses of energy and opens prospects for almost inertial-free control by combustion processes.

Calculations of three-dimensional stationary flows in lower parts of the tornado and of the tropical cyclone of middle intensity

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The three-dimensional non-stationary flows of ideal polytropic gas are mathematically designed in the conditions of action of gravity and Coriolis. For the system of equations of gas dynamics the initial-regional is put task, the decision of that describes a flow arising up at the smooth flow of gas through a surface vertical cylinder of the set nonzero radius in the vicinity of impenetrable plane of $z = 0$. It is well-proven that this task also is the characteristic Cauchy of standard kind problem and, on condition of analyticity of the initial datas, it has an only analytical decision. The analysis of the first coefficients of row showed on the degrees of z , that at beginning of radial flow into a cylinder at once there is circuitous motion of gas, involute in the North hemisphere in positive direction and in negative direction for the case of the South hemisphere. For the design of three-dimensional non-stationary underflow of such natural whirlwinds as a tornado and tropical cyclones are used initial segment of row, a questioner this analytical decision. The coefficients of initial segments of rows are numeral built at the decision of the corresponding systems of hyperbolic type.

3. Power Interaction with Matter

Accelerator driven high energy density science: Status of high-energy-density physics at FAIR and GSI

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High intensity particle accelerators like FAIR at GSI Helmholtzzentrum für Schwerionenforschung (GSI–Darmstadt) and the proposed HIAF facility in China are new tools to induce high-energy-density states in matter. The development of this field connects intimately to the advances in accelerator physics and technology. At Xi'An Jiaotong University we are starting a group that will build a low energy, high current ion beam facility for basic beam plasma interaction physics and will make use of existing machines at GSI–Darmstadt, the Institute of Theoretical and Experimental Physics in Moscow (ITEP–Moscow), and the Institute of Modern Physics (IMP–Lanzhou). A brief report on the Accelerator Facility (HIAF), under development in China will be included. The National Natural Science Foundation of China grants U1532263, 11505248, 11375034, 11205225, 11275241, and 11275238.

High energy density physics at the Facility for Antiproton and Ion Research

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High energy density physics (HEDP) including study of matter under extreme conditions of temperature and density is a developing multidisciplinary field that is expanding the frontiers of many scientific disciplines. HEDP cuts across many traditional fields of physical science, including astrophysics, cosmology, nuclear physics, plasma physics, laser science, and material science. HEDP, along with atomic physics, biophysics and materials research, forms one of the 4 major scientific pillars for the Facility for Antiproton and Ion Research (FAIR) presently under construction at the GSI site in Darmstadt. These pillars will utilize the unique capabilities of FAIR to grow and develop forefront scientific understanding through the first half of this century. Accessing warm dense matter (WDM) conditions in the laboratory presently utilizes a variety of techniques including shock drivers that are laser-driven, Z-pinch-driven or explosive-driven. These techniques reach pressures in the range of 1–10 Mbar and are well established. As an alternative, volumetric heating from highly penetrating photon (x-ray) sources and particle beams (electrons, ions) provide several advantages. This generates e.g. WDM in local thermodynamic equilibrium and with samples large enough such that these systems are relatively uniform and evolve on the ns to μ s time-scale. The use of heavy-ion beams at FAIR for creating WDM states offers a unique and complementary approach to the other WDM drivers. In the report there will be present the status of HEDP studies at FAIR (HED@FAIR) collaboration with experimental program that will be conducted at the dedicated plasma physics beamline in the APPA cave of FAIR.

Diagnostics of energy transfer in foils heated by petawatt laser pulses by x-ray absorption spectroscopy

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Absorption x-ray spectroscopy is proposed as a method for studying the heating of solid-density matter excited by secondary x-ray radiation from a relativistic laser-produced plasma. The method was developed and applied to experiments involving thin silicon foils irradiated by 0.5–1.5 ps duration ultra-high contrast laser pulses with intensities $(0.5\text{--}2.5)\times 10^{20}$ W/cm². The electron temperature of material at the rear side of a target is estimated to be in the range of 140–300 eV. The diagnostic approach accessed and enables the diagnosis of warm dense matter states with a low self emmissivity.

Ultra-intense K-shell emission from medium Z foils irradiated by optical femtosecond laser pulses with intensity higher than 10^{21} W/cm²

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We report about x-ray spectroscopy advantages in experiments at J-KAREN-P laser facility. The high-resolution x-ray diagnostic was applied to observe x-ray emission from dense laser plasma generated via ultra-intense ($I \gtrsim 10^{21}$ W/cm²) fs laser pulses irradiated thin stainless steel foils. For the first time, we demonstrate from high-intensity laser generated plasma that the highest temperature emission region had electron density reached a relativistic critical density value, which is of 30 times higher than the typically observed critical density for the laser wavelength. Kinetic modeling using code FLYCHK was provided to estimate main plasma parameters at the assumption of x-ray emission from different plasma zones.

Laboratory studying of matter accretion in young stars by means of x-ray spectrometry

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This paper aims the studying the accretion dynamics of young stars in laboratory. The experiments were conducted in laboratory LULI of Ecole Polytechnique in Palaiseau, France. In order to investigate the accretion dynamics in the laboratory we create a collimated narrow (1 mm diameter) plasma stream by imposing a strong ($B_z = 20$ T) external and uniform poloidal magnetic field onto an expanding high-power laser (1 ns duration, 10^{13} W/cm²) ablated plasma. Targets were made of thick CF₂ and mylar bulk. The stream ($v_{\text{stream}} = 750$ km/s, $T_e = 10\text{--}20$ eV) propagates parallel to the lines of the large-scale external magnetic field, onto an obstacle mimicking the high-density region of the star chromosphere. We observe in these experiments that matter, upon impact, is laterally ejected from the solid surface, then refocused by the magnetic field toward the incoming stream. Such ejected matter forms a plasma shell that envelops the shocked core. The parameters of both plasma core and shell were studied by means of spatially resolved x-ray spectroscopy [1] and Mach–Zehnder interferometry. The issue connected with opacity through shell plasma has been studied.

[1] Ryazantsev S N, Skobelev I Y, Faenov A Y, Pikuz T A, Grum-Grzhimailo A N and Pikuz S A 2015 *JETP Lett.* **102** 817–22

The study of linear inductive accelerator bremsstrahlung generation in two-pulse mode of operation

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The study of dynamic processes in optically opaque objects of high density is mainly carried out by the flash radiography method. One of the most prospective x-ray sources is linear inductive accelerator of electrons (LIA). As a result of intense electron beam focusing on the accelerator target, energy release exceeds vaporization and ionization threshold that leads to dense target plasma formation. Back-streaming plasma ions flux causes electrons beam defocusing. The study of focal spot evolution in one-pulse mode (pulse duration 180 ns) and two-pulse mode of operation (time delay between pulses from 2 to 20 μ s) is presented. The study shows that the first beam defocusing is caused by light surface molecules vaporization and can be minimize by target melting (pre-pulse). The second LIA pulse defocusing caused by supposedly target plasma formation after the first pulse was observed. The focal spot increasing time dependence was obtained. It was shown that diminished energy release of the first pulse leads to not so high the second pulse defocusing.

Compression and burning of direct drive targets under space-time inhomogeneous irradiation

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It is well known, that the optimal approach to realize compression and burning of laser targets is the usage of thin solid shells (ablator and DT-fuel) and spherical symmetry of their compression. The problem to achieve the most symmetric irradiation, and the laser energy absorption is a key one. An experience of the numerous theoretical and experimental investigations during last years [1–4] leads us to analyze again the possibilities of the direct drive laser ICF (inertial confinement fusion) approach, and to establish the possible limits of the symmetry violations, due to the different natural causes. At the present work we try to establish the effects due to the principal deviations from a symmetric case: geometry of irradiation, misbalance of the laser energy between the beams, slip of the beams, time non-simultaneity of the beams, and shift of the target from the camera center. We came to the conclusion, that it is possible [4] to get a considerable neutron yield (about 10^{18} – 10^{19}), and so, to reach an ignition of the thermonuclear fuel and to obtain a significant gain, about 10, using Nd laser at second harmonic with the energy about 2–3 MJ.

[1] Betti R and Hurricane O A 2016 *Nat. Phys.* **12** 435–48

[2] Doppner T, Callahan D A, Hurricane O A and *et al* 2015 *Phys. Rev. Lett.* **115** 055001

[3] Igumenshchev I V, Michel P T, Shan R C and *et al* 2017 *Phys. Plasmas* **24** 056307

[4] Belkov S A, Bondarenko S V, Vergunova G A and *et al* 2017 *J. Exp. Theor. Phys.* **124** 341–51

Kilojoule-level multifunctional laser system ELF-MEPHI

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Current concept of amplifying systems for inertial confinement fusion and extreme states of matter researches is oriented to four-pass amplification scheme. Energy characteristics of such systems are limited by the possibilities of intense radiation transporting by optical elements, accumulation of B-integral, limitation of the energy in the reverser amount. Repeating of the optical path with an imperfect quality of transport and amplification systems leads to an intensive accumulation of aberrations. In this case, the beam accumulates the overwhelming part of the energy at the last pass of the amplifiers only.

Amplification of laser radiation in the multiple saturation regime was proposed. The implementation of the new amplification scheme within the project of the multifunctional laser complex ELF-MEPHI (experimental laser facility) (NRNU–MEPhI) will: reduce the number of parts involved in amplifying and radiation transporting; reduce divergence; increase stored energy extracting efficiency, increase functionality of the installation; increase the frequency of experiments; improve ergonomics; reduce the price of channel and operating costs. As part of multifunctional laser complex development, it is proposed to develop an installation with adjustable time, spectral and energy parameters. It consists of two laser channels for generating two radiation pulses in one experiment with controlled time delay: a nanosecond pulse with an energy of up to 8 kJ (duration 3–10 ns, power density up to 10^{16} W/cm²) and a subpicosecond pulse of energy up to 300 J (duration 1.0 ps, power density up to 10^{20} W/cm²).

Diagnostic system for measuring mass velocity of matter under the influence of intense laser radiation

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The paper presents the diagnostic system for velocity measurements of reflecting objects in high energy physics experiments. The principle of continuous velocity measurements based on the Doppler frequency shift analysis of a probe monochromatic wave reflected by the moving surface of the sample. The system is designed to measure speed in the interval of 5 to 50 km/s and consists of 3 separate parts: optical stand with interferometers, probe laser for target illumination and control computer. The back side of target is illuminated by probe laser beam at a wavelength of 660 nm. The diffused and reflected probe light is collected by a lens and injected into the optical system. Optical system based on two time-imaging Mach–Zender unequal path interferometers, that form a vernier measuring system. Registration is performed by streak-cameras with time resolution about 10 ps. Magnification of optical system is variable and allows to make experiments with different-size field of view on target (in range of 0.3–0.6 mm). Also, system has passive registration channel for target luminescence measurements with the same spatial and time resolution as interferometer channel data. Probe light source is a pulsed Nd laser at a wavelength of 660 nm (2nd harmonic of 1320 nm). Probe laser consists of semiconductor master oscillator and regenerative amplifier. This scheme allows obtaining the pulse with energy of 30 mJ, time duration 100 ns with the frequency of 10 Hz.

Studying the damage effect of high-power coherent terahertz pulses on living cells

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The problem of human safety at working with THz radiation become especially urgent now, when studies on creation of high-power sources of coherent pulsed terahertz radiation succeeded. This makes it possible to predict widespread implementation of such THz equipment for solving dual-purpose tasks, including remote detection of hazardous substances, in the nearest future.

The issue of safety of THz radiation for living objects (from the molecular to the organism level) is still a matter of disputes and requires further investigations. A source of THz radiation of record-power, based on the unique femtosecond chromium-forsterite laser system is created in JIHT RAS. The source with such parameters was used for the first time to investigate the damaging effect of radiation on living bio-objects in scope of further developing safety standards and means of protection.

The propagation effects in ultrafast nonlinear electro-optical modulation in thin film on a substrate

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At present, table-top sources of terahertz radiation (THz) provide ultrashort pulses with 1 ps duration and peak amplitude up to several MV/cm. Such single-period pulses can be used as a unique means for all-optical ultrafast control of the material properties by the electric field of these pulses. The effects of ultrafast THz modulation of the sample properties are studied by a “pump-probe” technique, in which THz pulse is used as a pump, and a femtosecond optical pulse is used as a probe. The rotation of polarization, generation of the second optical harmonic, etc can be observed. In fact, these effects are ultrafast analogs of electro-optical effects.

When interpreting the results of observations, problems arise related to the effects of the propagation of a terahertz pulse in a medium: echo effects, interference effects, the phase change effect as a function of the thickness of the medium layer, etc.

In this paper, the propagation of short optical and terahertz pulses through a structure consisting of a noncentrosymmetric film on a centrosymmetric substrate is considered. With the spatial and temporal overlap of these pulses in the film region, the effect of electro-induced second optical harmonic generation is observed. It is shown that the difference in the group velocities of these pulses leads to a non-mirror dependence of the transient nonlinear-optical response upon a mirror image of the film/substrate structure relative to its surface.

The work has been performed with a financial support from the Russian Science Foundation (project No. 16-12-10520).

Ablation of molybdenum induced by femtosecond laser

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Molybdenum is a high-strength refractory structural material widely used in industry, whose behavior at high temperatures causes considerable experimental and theoretical interest. In this paper we present the results of experimental studies of the behavior of molybdenum at high temperature (3–10 kK) and pressure (50–100 Kbar) produced by the action of laser pulses with a duration of 40 fs at the intensity of 10^{12} – 10^{13} W/cm². An absorbed fluence at the ablation threshold and the dependence of the crater depth on the intensity of the laser pulse were measured. Also morphology of the irradiated surface by atomic force and scanning electron microscopy was investigated. A temporal dynamics of the surface layer expansion was measured by ultrafast interferometry with a picosecond temporal resolution.

The results of the research are of fundamental interest for the development of condensed matter physics, testing of hydrodynamic and molecular dynamics calculations and development of precision methods for laser processing of thin-film materials for microelectronics.

Simulation of single-, double- and multi-pulse laser ablation of metals

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We present some results of one-dimensional hydrodynamic modeling of laser ablation of metals by femtosecond laser pulses in regimes of single- [1], double- [2] and multi-pulse irradiation [3]. Effects of plasma shielding, suppression of ablation and increase of ablation efficiency are investigated and discussed.

This work was supported by the Russian Science Foundation, grant No. 16-19-10700.

- [1] Povarnitsyn M E, Itina T E, Sentis M, Khishchenko K V and Levashov P R 2007 *Phys. Rev. B* **75** 235414
- [2] Povarnitsyn M E, Fokin V B, Levashov P R and Itina T E 2015 *Phys. Rev. B* **92** 174104
- [3] Povarnitsyn M E, Levashov P R and Knyazev D V 2018 Simulation of ultrafast bursts of subpicosecond pulses: In pursuit of efficiency, submitted to *Appl. Phys. Lett.*

Simulation of nanoparticles formation during femtosecond laser ablation of aluminum in water

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Various colloid mixtures of nanoparticles have a lot of applications in science and technology. These mixtures can be produced efficiently by a femtosecond laser pulse action on a metal target immersed into a liquid.

We developed a Hybrid Continuum-Atomistic Model [1] which allows us to describe the mechanisms underlying the laser ablation in these fast technological processes. This model is based on approach [2], and it can represent the fragmentation of a metal both in solid and liquid phases under the influence of double and multiple laser pulses.

In our model [1] the ion subsystem is described by the equations of molecular dynamics, and the energy equation for electrons is solved to calculate the evolution of the electronic subsystem. Absorption of laser radiation is calculated by solving the Helmholtz equations, and wide-range models are used to determine the dielectric constant, electronic thermal conductivity, and electron–ion exchange [3].

We apply our model for describing of the evolution of the nanoparticles formation during the laser ablation of an aluminum target, including ablation into liquid water under pressure.

We analyze the evolution of a two-phase liquid–vapor mixture, the mechanisms of nanoparticles formation during such evolution, and the size distribution of nanoparticles.

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Ablation into water: Fragmentation of metal via Rayleigh–Taylor instability

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Laser ablation of metals in liquid is very different from ablation in vacuum. In contrast to the last the corresponding processes are still poorly understood. We show that to produce metal nanoparticles the laser absorbed energy should few times overcome the ablation threshold for the contact with vacuum. Then the temperature in the heated layer increases above the critical point. Our analysis of the flow as whole with a strong shock propagating in liquid and with a rarefaction wave inside the metal target demonstrates that the contact between metal and liquid, both in their supercritical states, is hydrodynamically unstable. The instability is of the Rayleigh–Taylor type. Its dynamics is important for generation of metal droplets freezing soon into solid nanoparticles.

Ultrashort pulse action onto thin film on substrate: Shock propagation in substrate

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Thin films located upon supporting substrates are important class of laser targets for surface nano-size modification, e.g. for plasmonic or sensoric applications. There are many papers devoted to this problem. But all of them are concentrated on dynamics of a film, paying small attention to substrate. In these papers the substrate is just an object absorbing the first shock. Here we present another point of view directed onto dynamics of a substrate. We consider (i) generation of a shock wave (SW) in a supporting substrate, generation by impact of a film–support contact on supporting condensed medium; (ii) transition from one to two-dimensional (2D) propagation of SW; (iii) we analyze lateral propagation of the SW along a film–support contact; and (iv) we calculate pressure in the compressed layer behind the decaying SW. This positive pressure acting from substrate to the film accelerates the film in direction to vacuum. Above some threshold, velocity of accelerated film is enough to separate the film from support. In the cases with large energy absorbed by a film, the circle of separation is significantly wider than the circle of high heating around the focal laser spot on film surface. Absorbed laser heat exponentially decays around an irradiated spot as $\exp(-r^2/R_L^2)$, where R_L is radius of Gaussian beam. While the law of decay for the 2D SW in substrate is the power law. Therefore in the mentioned cases of powerful laser action the edge of a separation circle is driven by SW in support.

Numerical simulation of the holes formation in thin metal films under femtosecond laser irradiation

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Investigated is the process of surface nanostructures formation due to femtosecond laser irradiation of the thin golden film, deposited on the thick glass substrate. Depending on adsorbed fluence, the unexpectedly rapid growth of the nanostructures diameter can be observed. Two-dimensional hydrodynamic model and code are presented for investigation of the underlying mechanism. Considered are the stages of propagation and spherisation of the arising shock wave, which lead to layer-by-layer delamination of the film from the substrate and form the holes. Estimates of the hole diameter are made. The data obtained correspond well with the experimental results.

Two-temperature kinetic coefficients of liquid aluminum in the conditions arising under the action of a femtosecond laser pulse

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Resistivity and thermal conductivity of aluminum in the liquid phase are calculated by using Ziman approach in the states, typical for the ablation process under the action of femtosecond laser pulse onto the metals. These states include the liquid metal of near normal density with different electron and ion temperatures at the early stage and also states with density and temperature close to their critical values. Electronic spectrum is found by the density functional method, the structural factor of a liquid is determined by the classical molecular dynamics method with the use of the interatomic potential via the “embedded atom” model. Relaxation time approach is used to calculate electrical conductivity and a resistivity as a reverse to it, and thermal conductivity is found by the use of Onsager coefficients in the relaxation time approach. The influence of various types of screening of electron-ion interactions onto the results of the theoretical calculations of resistivity and thermal conductivity is investigated.

Cluster phenomena caused by metallic ablation

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Laser ablation of different metallic surfaces in superfluid He leads to formation in liquid bulk of different exotic clusters (see for e.g. [1–3]). In this line the most impressive are the different types of quasi-one-dimensional, visible dendrites with metallic conductivity. In this presentation the possible scenario of dendrite chain growing in presence of external electric field is discussed.

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Synthesis of carbon-encapsulated molybdenum nanoparticles using forth harmonic pulse Nd:YAG laser

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Carbon-encapsulated molybdenum nanoparticles were synthesized by laser-assisted photolysis of gaseous precursors. Gas mixtures containing various hydrocarbons and molybdenum hexacarbonyl vapor diluted in argon were irradiated with a nanosecond pulsed ultraviolet laser at room temperature. Particle samples were analyzed by transmission electron microscopy, electron microdiffraction, energy-dispersive x-ray spectroscopy, and high-angle annular dark-field scanning transmission electron microscopy techniques to provide nanoparticles morphology and composition. The influence of hydrocarbon type, its mole ratio, and number of uv laser pulses on resulting carbon-encapsulated molybdenum nanoparticles was investigated. The synthesized nanoparticles were heavily aggregated and consisted of Mo-based cores surrounded with carbon material. The hydrocarbon type did not cause any effects on nanoparticle formation and growth processes. The increase of hydrocarbon mole ratio in the precursor mixture led to increase of carbon content and decrease of Mo-based core size in the samples. The increase of uv laser pulses number appeared to cause the enlargement of Mo-based cores in carbon-encapsulated molybdenum nanoparticles.

Laser ablation thresholds for optical and x-ray lasers

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With the use of two-temperature (2T) hydrodynamics, the effect of radiation from an optical laser and an x-ray laser with the same fluence was compared. The penetration depth of x-ray radiation is larger than that of optical radiation. One would expect that the ablation threshold will be greater for the case of an x-ray laser. Calculations show that after the 2T stage, the temperature profiles under the action of an optical laser and an x-ray laser with a pulse duration that is greater and smaller than for an optical laser are practically the same. As a result, the threshold in the x-ray case is not higher than in the case of optical radiation.

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Polycapillary system fabrication and their transparency for femtosecond laser pulses

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Currently hollow core photonic crystal fibers are widely used for spectroscopy, sensors and communication systems. Structured air channels causes light confinement in hollow core due to formation of band gaps and dispersion effects. It allows to achieve surface enhanced Raman scattering for metal vapor deposited and silica coated structures. We present experimental results for laser pulse propagation through microstructured optical fibers fabricated at our laboratory. We have made estimation for femtosecond Ti:Sapphire laser with average 800 mW power. The energy 10 nJ per impulse with beam focusing to spot size $1.3 \mu\text{m}$ gives electric field with tension $|E| = 1.2 \text{ V}/\text{\AA}$. This field is enough to produce ionization of inner surface atoms and surface plasmons generation. Also temperature dependence of adsorption spectra is investigated as was done in [1].

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On factors controlling emittance of electron bunches accelerated in guiding structures

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Ensuring low value of emittance of electron bunches accelerated in guiding structures is crucial for the concept of a multistage laser electrons accelerator. In the present work we make analytical study of the factors, which determine the value of normalized emittance of electron bunches in guiding structures: plasma channels and capillary waveguides, for different ratios of guiding structure and laser pulses characteristic transverse sizes. In the case of small initial value of normalized emittance much below than its self-consistent (for given transverse size and injection point) final value, simple formula is derived, which permits one to estimate this final value for electron bunches with arbitrary longitudinal length, accelerated in fitted plasma channel.

Qualitative analyses is conducted and it is shown that the emittance is determined substantially by longitudinal and transverse sizes of the accelerated electron bunch, its phase of injection into accelerating wakefields and by the accuracy of laser pulse focusing into a guiding structure, which determines the quality of accelerating wake fields. In particular, it is shown that the low emittance requirement imposes an order of magnitude more severe restrictions on the accuracy of laser pulses focusing [1] into guiding structures than the requirements of high energy gain, of low energy spread and the conservation of a large number of trapped and accelerated particles in an accelerated electron bunch.

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

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Study of the thermomechanical ablation crater on the sodium chloride surface

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With a terawatt titanium–sapphire femtosecond laser system [1], pulses at $\lambda = 800$ nm with a duration of 40 ± 2 fs produced a crater on the sodium chloride surface [2]. First, estimating the depth of the crater (h), the fringe shift technique was used [3].

Observations showed that for dielectrics it could be estimated that the depth of the crater exceeded 100 nm, in comparison with metals, where h is tens of nm [1].

According to the measurements, using an atomic force microscope, for a pulse with the power 4.1 GW, the depth of the crater for sodium chloride was 1.4 μm . In aluminum, according to [4], at the same pulse parameters, we expect h to be of the order of 100 nm. This work was supported in the framework of the base part of the Russian DES government task KBSU for years 2017–2019 (project number 3.8382.2017).

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X-ray photoelectron spectroscopy in research of potassium bromide after laser treatment

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The effect of laser radiation on the ionic crystal surface was carried out using a terawatt titanium–sapphire femtosecond laser system of the Laser Femtosecond Complex Center of Collective Use of Unique Scientific Equipment of the Joint Institute for High Temperatures, Russian Academy of Sciences [1] and a power density in the treatment spot attained 90 TW/cm^2 [2]. Femtosecond laser pulses at a wavelength of 800 nm leads to optical damages on the sample surface. To analyze the effects of exposure to the laser used x-ray photoelectron spectrometer “Termo Scientific K-Alpha”, where the vacuum was of the order of 10^{-9} mbar. In the case of study of the surface elemental composition, the concentration of the sample components was determined with an accuracy of $\pm 0.3 \text{ at}\%$, the energy of the electrons at the site was up to $\pm 0.2 \text{ eV}$ [3]. Explore the surface in the spot of damage and outside it, before and after cleaning the surface the ion bombardment with argon ions of the crystal. Comparative analysis of XPS spectra showed that in the case of potassium bromide, high-intensity laser irradiation significantly affects the surface of an ionic crystal. This work was supported in the framework of the base part of the Russian DES government task KBSU for years 2017–2019 (project number 3.8382.2017).

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Fracture hydrodynamics of fused quartz in the process of volumetric heating

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Silica-based optical fiber is convenient target for studying the solid density plasma interaction with cold silica in the process of laser-induced fracture. The experimental study shows that the basic mechanism of medium destruction is the localized optical breakdown leading to the formation of hot plasma. Hot plasma expands and causes corresponding deformation of the solid medium. As a result hydrodynamic motion arises both in solid medium and plasma that causes strain of the medium in the vicinity of interfacial boundary. Finally the solid medium begins to be fractured. This work studies numerically the development of the wave processes in the vicinity of interfacial boundary which was formed due to the local optical breakdown induced by the laser impulse. The results allow us to get a clear interpretation of the processes involved in the solid medium fracture in two different regimes. The first regime concerns the slow propagation of the absorption front via the heat transfer from the hot plasma to the cold solid quartz. The second one concerns the transonic propagation of the absorption front. It is shown that in both cases the fracture occurs as soon as the expanding hot medium pushes the solid medium boundary. Herewith, one can observe the formation of compression wave in the solid medium followed by the rarefaction wave. This process is repeated in time that is related with the consecutive phase front propagation into the solid matter. The characteristic wave length of this process is estimated as $2.35 \mu\text{m}$ that correlates well with the characteristic size of small-scale fragments observed experimentally.

The work was funded by Russian Foundation for Basic Research (grant No. 17-08-00574)

The heat field during laser ablation at high temperatures

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The authors [1–3] were performed numerical experiments on laser ablation of glass composites. The heat equation was solved by the moments method. After researching “subthreshold” approximation $l \ll 1$ and $T_s \ll T_a$ (l is the heating typical size, T_s is the surface temperature, T_a is the typical ablation temperature), the task was to consider another boundary approximation, when $T_s \gg T_a$:

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

where $T = T_s - T_0$ and T_0 is initial value, α, κ, c, ρ are the target parameters and I_s is the intensity of the radiation on the front of the ablation.

This task, although different from the problems considered by several authors [4], is important for studies at extreme values of energy density of the laser radiation. Being a mathematically correctly obtained solution, this system gives you the ability to build interesting hypotheses of the interaction of radiation and matter.

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Possible utilization of space debris for laser propulsion

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Laser propulsion perspectives become more realistic with the development of laser systems, necessity to resolve space debris problem and to perform high specific impulse interplanetary flights. Unlike others, laser thrusters can use virtually any type of fuel by turning it into plasma, this provides great abilities for harvesting working medium in space instead of bringing it from the Earth. This and ability to reuse external laser source intensively could save a lot of money and broaden abilities for thrusterless small satellites (nano- and pico-especially) and formations of those.

We considered several options for spacecraft to use space debris (including out-of-use satellites, launcher stages) material as a fuel for laser-induced jet. Evaluated possible mass consumption, thrust, velocity and energy efficiency performance, as well as optimal laser impact regimes, demanded Δv and time scale for different missions. For example, 100 mJ nanosecond DPSS (diode-pumped solid-state) laser (with net electrooptical efficiency of cca 10%) could ablate 1 kg of iron in 4 days at 1 kHz rate with a mass averaged speed of cca 10 km/s. Velocity Δv is enough to make 1 tonn LEO (low earth orbit) object burn in the atmosphere can be produced by ablation of 10 kg in this way. Our findings appear to be rather realistic in terms of the state-of-art launchable lasers, surface scanning systems and cost effect.

Theoretical and experimental studies of laser heating of low-molecular polymer styrosil

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Regularities in the continuous laser-induced dissipation and ablation of the low-molecular polymer styrosil with various additives have been studied. An experimental facility consisting of fiber ytterbium laser with an operating wavelength of $\lambda = 1.07 \mu\text{m}$ and procedures to measure the effect of laser irradiation were developed. Experimental data on the mass losses of the sample, luminance temperature of its front and temperature of rear surfaces were obtained. A mathematical model of the continuous laser-induced thermal destruction of the polymer was developed. This model was implemented and calculations were done both in the one-dimensional software approximation in own software product and in the software suite LOGOS designed for three-dimensional engineering simulations. Verified against the experimental data obtained, our model allowed us to calculate the values of mass losses, depth of thermal destruction, luminance temperature of its front and temperature of rear surfaces with maximum relative error below 10%. As a result of the studies, we established the effect of incident laser power density on the space-time structure of the temperature field and revised the parameters of laser light inducing fast losses of the carbon residue. These results can be used to optimize the parameters of the polymer.

Femtosecond laser nano and microstructuring for heat transfer enhancement

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The need for new functional surfaces with enhanced heat transfer is driven by the continuing increases in power dissipation of electronic devices. The spray cooling technology appears to offer the best balance of high heat flux removal capability and fluid use, while the functional surfaces with enhanced wettability and heat transfer characteristics are still in great demand. The key factors in controlling interfacial phenomena, including wettability and surface heat transfer, are morphology and physicochemical properties of a surface. The study shows the tremendous effect of femtosecond laser surface nano and microstructuring on wettability, evaporation rate and the Leidenfrost temperature. The enhanced wetting behavior stems from hierarchical surface morphology characterized by a microgrooved pattern, extensively covered by flake-like nanostructures. As a result, heat transfer characteristics of heated surfaces could be significantly improved that is of great importance, particularly to spray-cooling technologies and further development of power engineering systems and electronic devices.

Thermalization of laser excited aluminium nanoparticles: Wave packet molecular dynamics

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In recent times, nanoparticle (NP) interaction with ultrashort laser pulses has been a subject of significant interest due to several unique properties discussed in several theoretical and experimental works [1–3]. Among the most interesting questions is the possibility to obtain plasma with near-solid density (warm dense matter) by use of ultrashort laser pulses of TW/cm² fluences.

As non-equilibrium warm dense matter is a very complicated object for a theoretical description in this work we use *ab initio* molecular dynamics to investigate relaxation processes in Al NPs. Unlike density-functional-theory or classical methods, wave packet (w.p.) molecular dynamics provides a unique possibility to describe non-adiabatic effects and at the same time is not very computationally demanding. We apply the eFF (electron force field) w.p. model to different Al nanoclusters after an intense laser excitation. In this method electrons are represented as floating Gaussians and interactions between electrons are restricted to pairwise components only. Recently [4], this method has been successfully used to study the response Al NP on irradiation by short laser pulses. In this report, we present a further investigation of thermalization processes in laser excited aluminum NPs.

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Modeling of thermal and non-thermal melting of silicon irradiated with femtosecond laser pulse

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Modeling of fs-laser damage formation is a nontrivial task, requiring description of the atomistic structure of material, its basic mechanical properties and nonadiabatic electron dynamics (electron–electron relaxation, scattering of fast electrons on ions, secondary ionization and cascading, covalent bond weakening) within a single framework. Here we study the process of silicon relaxation after fs-laser irradiation using first-principles-based electron force field (eFF).

Depending on the amount of energy deposited into the electron subsystem there can occur two scenarios of lattice melting in covalently-bonded semiconductors: thermal and non-thermal melting. Thermal regime is characterized by direct transfer of energy from excited electrons to ions via the process of electron-ion relaxation. Non-thermal regime occurs when excited electrons are transferred from the valence to the conduction band, changing the potential energy surface between atoms and reducing the energy of bonding interactions between them, which leads to a fast atomic relocation. Non-thermal melting requires higher levels of deposited energy and typically takes place on the timescale of several hundred femtoseconds—much faster than the thermal melting. In this talk we discuss processes of energy transfer from electron to ion subsystem in silicon, showing the dependence of electron-ion coupling parameter on the level of deposited energy and analyse the influence of the potential energy surface perturbation on the ion dynamics. The work is supported by the Russian Science Foundation (grant No. 14-50-00124).

Nonlinear resonance interactions of laser beam with dense atomic vapor

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An atomic vapor of a metal can be considered as a dense resonance gas, if a volume of cubed resonance wavelength includes more than one atom [1]. At such experimental conditions, the dipole–dipole interaction induced broadening of a resonance atomic transition can be a dominant contribution to a spectral width of the resonance atomic transitions to compare with a natural width or even Doppler width of these transitions. In the excited dense vapor, the interatomic dipole–dipole interactions can be strongly modified [3].

Different coherent and incoherent nonlinear optical effects can be observed in dense resonance gases [1, 3]. We report recent results of our experimental studies: self-focusing and self-trapping propagation of laser beam in a dense rubidium vapor, nonlinear selective reflection of laser beam from a dense rubidium vapor. Our results can be used to model an interaction of intense optical radiation with resonance medium and plasma.

The work is supported by the Presidium RAS (basic research program “Investigation of Matter in Extreme States” headed by V E Fortov).

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The use of molecules and solids to search for a new physics

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“New physics” is physics beyond the standard model (SM), i.e. the theoretical developments (extensions) needed to explain the deficiencies of SM. One of most intriguing problems here is time-reversal (T) asymmetry of the weak interactions that is suppressed in SM but is predicted up to ten orders of magnitude higher in popular SM extensions making such effects observable experimentally. The most promising objects for such experiments now are heavy-atom diatomics [1]. The best upper limit on the electron electric dipole moment (eEDM), $|d_e| < 9 \times 10^{-29}$ e cm, was set in 2013 with the beam of ThO molecules in the metastable $H^3\Delta_1$ state [2]. The nonzero eEDM means violation of both T and P (space parity) symmetries. The current eEDM limit is on the level of predictions of the SM extensions. However, the success of such experiments depends on the progress in theoretical prediction of molecular properties and the T,P-odd effective Hamiltonian parameters [1, 3]. Not only the parameters which cannot be measured, but the hyperfine structure constants and dependence of g -factors of the rotational levels on external fields, spectroscopic properties, etc are of interest [3]. Other properties of T,P-odd interactions induced by both electron-nucleus and nuclear (Schiff and magnetic quadrupole) T,P-odd forces [1] can also be studied. The goal of the talk is to review the experiments to search for T,P-odd effects and our theoretical studies of both spectroscopic and T,P-odd characteristics for heavy-atom diatomics, which are of particular interest to search the T,P-odd effects.

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Propagation of a polarized electromagnetic wave in two-dimensional photonic crystal with a microcavity in a central air channel

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Polycapillary optics technologies are developing in x-ray optical systems laboratory of KBSC RAS. High quality of our polycapillary fibers produced by stretching and femtosecond laser allow us to investigate optical effects occurring in two-dimensional photonic crystals. We present the new method for calculating propagation of a polarized electromagnetic wave in polycapillaries with central hollow defect. The method is similar to that used for the calculation of the band structure of the crystal lattice with defects. The interaction with a microcavity inside the central defect of the polycapillary was investigated for the electromagnetic-radiation modes obtained.

Temperature effect of radiation for above-100-GeV electrons in oriented germanium crystal

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The electrostatic field strength of atomic chains along the major crystalline axes can be about $\sim 10^3$ eV/Å. The Schwinger's invariant strong field parameter χ for above 100 GeV electrons incident on crystals oriented along this directions can be of the order of unity and electromagnetic strong field effects can take place [1, 2]. Here

$$\chi = \frac{e\hbar}{m^2c^3} |F_{\mu\nu}p^\mu|,$$

where $F_{\mu\nu}$ is a field tensor of the crystal axes, p^μ is the 4-momentum of an electron, e and m are electron charge and rest mass.

We have calculated the intensity radiation spectra of 150 GeV electrons incident on germanium single crystal oriented along $\langle 110 \rangle$ crystallographic direction. The invariant field parameter in this case $\chi \approx 1$. The effect of multiphoton gamma radiation takes place under such conditions [3, 4]. For relatively low electron energies, less than few GeV, the temperature effect was studied earlier [5].

Our calculations are based on solution of the cascade type kinetic equations [3]. It has been shown that the intensity spectrum in its maximum increases by a factor of 1.5 with decrease of the crystal temperature from 293 to 100 K.

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Wide-range high-resolution LiF crystal x-ray detector calibrated with synchrotron radiation

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Today the lithium fluoride detectors are becoming increasingly popular in experiments on generation and characterization of the x-ray radiation including XFEL. Our work is devoted to an experimental determination of the metrological properties of LiF crystals used as fluorescent x-ray detectors. An experimental calibration was carried out by using experiments on synchrotron sources. These experiments allowed us to determine the sensitivity limit and the function of the crystal response to radiation in a wide dynamic range.

The spatial resolution of LiF is limited by the size of the secondary electron cloud. The dependence of the radius of a such cloud on the x-ray radiation energy was theoretically calculated. In this work, we also compared the theoretical and experimental data in the photons energy range 5–20 keV.

Capture and acceleration of electrons by the ultrarelativistic wakefield

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Modeling results of the external injection of electrons into wakefields excited by ultrarelativistic proton bunch in plasma are presented. Electrons motion is described by the system of relativistic dynamic equations [1]. Initial parameters of the plasma and the proton bunch are similar to the currently being carried out experiment AWAKE (Advanced Wakefield Experiment) at CERN [2]. Characteristics of the accelerated electron bunch (percentage of captured electrons and energy dispersion) are studied for the different injection angles to the wake wave propagation direction [3] and for different initial parameters of injected bunch. The optimal for capture area of the wake wave is defined. The research was carried out with support of Russian Science Foundation (project number 14-50-00124).

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The influence of the laser pulse selffocusing on the injection and acceleration of electrons in the plasma wake fields

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The wake waves in plasmas generated by high intensity laser pulses are of interest for acceleration of electrons to high energies. The creation of high-energy electron sources for injection into a laser-plasma accelerator was studied in [1, 2]. The aim of this work is to study the effect of self-focusing of a laser pulse on the injection and acceleration of electrons in the plasma wake fields. The laser pulse energy and the plasma density distribution were selected in accordance with the data [2]. Calculations were performed using the 3D particle-in-cell method [3]. The length of the laser pulse equals to 15 μm (45 fs), the focal spot radius at the level $1/e^2$ equals to 8.4 μm , the intensity at the focus equals to $9.4 \times 10^{17} \text{ W/cm}^2$. The density distribution of the plasma is Gaussian, with $n_{\text{max}} = 6.6 \times 10^{19} \text{ cm}^{-3}$. When the laser pulse in the process of its propagation in plasma reaches the region where the pulse power exceeds a critical value for self-focusing, the laser pulse is self-focused and a steepening of the leading edge of the pulse increases. These processes lead to self-modulation instability, generation of a wake plasma wave, to injection and acceleration of electrons. The maximum energy of electrons approaches 8 MeV that agrees with [2].

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Loading effect in trapping and acceleration of short electron bunches in laser wakefields

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The processes of trapping and acceleration of short electron bunches externally injected into the wakefields generated by intense femtosecond laser pulse in a plasma channel are analyzed and optimized. The influence of the beam loading effect (self-action of the bunch charge) to the finite energy and the energy spread of the accelerated electrons are investigated. The limitations to the charge of accelerated electron bunch determined by the requirement of a small width of the electron energy distribution of the bunch are found.

Matched conditions for multi-stage laser wakefield acceleration

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One of the promising scheme based on laser-plasma interactions, which is suitable for high-energy physics experiments, is multistage acceleration. In spite of technical issues the possibility of acceleration in two stages coupling by a plasma mirror has been already demonstrated [1]. In this work, a multistage acceleration of polarized electrons was considered, such that in the accelerating stage the electrons moved in the wakefield generated by intense laser pulse in plasma channel [2]. The purpose of this work was to investigate methods for preservation of the electron beam quality during acceleration. It was shown that matching a beam with a focusing force acting on electrons in plasma channel allows to prevent the growth of emittance and depolarization within accelerating stage. For efficient transport of particles between stages, the channel density linearly increased at the entrance and decreased at the exit from the stage, while the radius on the contrary decreased at the entrance and increased at the exit from the channel [3]. Such a scheme with the smooth entrances and exits should provide quasi adiabatic changing of emittance. The influence of this approach on the evolution of beam characteristics during interstage transfer was considered and the optimal parameters of the channel radius and density were proposed.

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Generation of attosecond electron bunches upon laser pulse propagation through a sharp plasma boundary

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Investigation of the generation of short electron bunches when a relativistic-intensity laser pulse propagates through a sharp plasma boundary has been studied [1]. Numerical simulation has demonstrated that the generation of electron bunches by a laser pulse is a consequence of multithread motion of the electron component of plasma. In certain conditions, such a motion can be presented in the form of mutually intersecting trajectories of plasma electrons, each electron being initially a plasma oscillator excited by laser pulse, which executes free oscillations around the initial position, which this electron occupied prior to the action of the laser pulse. Intersection of the trajectory of the plasma oscillator with that of the neighbouring oscillator results in self-injection of this electron into the wake wave produced by the laser pulse, which is the physical mechanism of generating an electron bunch. Simple formulae are obtained for estimating the duration of the electron bunch and the energy spread of bunch electrons after the process of the bunch formation terminates. It was found that the electron bunch duration may be of the order of several tens of attoseconds at the relative spread of the electron energy less than 10%.

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Hot electron generation for high-energy-density diagnostics

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Diagnostics of matter in high-energy-density states can be implemented based on laser–plasma interaction. Development of laser plasma electron sources able to produce large electron charges of about 10 nC with high energies of about 100 MeV and with low divergence of electron flow is of interest. In the present work, the interaction of the high-intensity laser pulse with the foam target was studied as a possible candidate for the source.

Previous numerical simulations showed that the foam with near-critical density is a perspective material for high-energy-density diagnostics and allows to obtain a large number of electrons with high enough energies. The main accelerating mechanism is assumed to be an energy gain under the action of the ponderomotive force of the laser pulse. During the interaction, self-focusing of the laser pulse takes place and the ponderomotive force grows. The effect of self-focusing explains the generation of particles with gradually increasing energies for the bulk of them. However, some number of electrons has energies above the ponderomotive one. Besides, the mechanism of non-adiabatic energy gain by particles is not clear.

In this work, electron trajectories were analyzed to find out the reasons for the irreversible energy gain. Several mechanisms were considered to explain the generation of particles with high energies beyond the ponderomotive energy such as direct acceleration in the laser field and acceleration in combined laser and plasma fields.

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Characterization of the hot electron energy distribution in the intense laser interaction with metal targets

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In experiments at the PHELIX laser facility, absolute measurements of the K_α radiation yield and measurements of bremsstrahlung emission by the radiation attenuation and half-shade methods were carried out under exposure of silver targets to laser pulse with an intensity of 2×10^{19} W/cm². To deduce parameters of the hot electron spectrum, we have developed semi-analytic models of generation and measurements of the x-rays. A two-temperature hot electron energy distribution has been revealed. Obtained temperatures are in agreement with the values predicted by kinetic simulations of the cone-guided approach to fast ignition. It is shown that electrons with a temperature of the order of the ponderomotive energy of 1.66 MeV are generated in a low-density preplasma, and electrons with a lower temperature of 130 keV are generated due to laser interactions with the plasma of subcritical density. We have obtained relatively low conversion efficiency of laser energy into the energy of hot electrons, directed into the target, of about 2% at a relatively low contrast ratio of a nanosecond amplified spontaneous emission of 10^6 . The colder electron component contains approximately 60% of the absorbed energy. It is shown that the assumption about a single-temperature hot electron energy distribution with the slope temperature described by the ponderomotive scaling relationship, without detailed analysis of the hot electron spectrum described here, strongly overestimates the laser-to-electron energy-conversion efficiency. In particular, the conversion efficiency of laser energy into the high-temperature component of the hot electron distribution can be thus overestimated by an order of magnitude.

The dipole structure of terahertz radiation by laser irradiation on clusters

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The theoretical description of radiation of terahertz (THz) waves is developed for laser-cluster interactions with allowance for the dipole emission mechanism. The excitation of THz fields in a cluster under the ponderomotive effect of laser radiation on free electrons is considered. The angular, spectral, and energy characteristics of THz radiation at large distances from the cluster in the wave zone were studied. It is shown that for a underdense cluster plasma there are sharp maxima in the emission spectrum at the frequencies of the dipole and quadrupole oscillations of the plasma sphere. With an increase in the density of free electrons, these spectral lines gradually disappear, and instead of them, in the case of a overdense electron concentration, a broad maximum is formed at a frequency comparable to the reciprocal of the laser pulse duration. It is shown that for small cluster sizes in the regime of frequent electron collisions, the angular energy distribution has a dipole structure, and THz radiation emits mainly at an angle 90 degrees with respect to the propagation direction of the laser pulse. The total energy of THz radiation was calculated and its dependence on the density of free electrons was investigated. It is shown that the energy of THz radiation has the maximum value in a dense cluster plasma under resonance conditions, when the frequency of laser radiation coincides with the eigenfrequencies of the dipole and quadrupole modes of the plasma sphere. It is established that the dipole mechanism of THz emission is prevalent for clusters with small dimensions under conditions of frequent electron collisions.

Determination of the absolute intensities for x-ray spectral emission lines of multiply charged silicon ions in a relativistic laser plasma

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At present, x-ray spectroscopy methods are widely used in fundamental research in the study of atoms, molecules and macroscopic bodies formed from them. Due to the imperfection of spectrometric instruments and the peculiarities of carrying out each particular experiment, the recorded data requires correct interpretation. Elimination of spectrum distortions associated with errors in measuring equipment by taking into account the hardware function of the spectrometric path is an actual problem, since most x-ray spectral diagnostic methods are based on an analysis of the characteristic features of the recorded spectrum. The result of this work is the obtaining of spectra with real values for the number of photons. Data on the relative intensities of the spectral lines are sufficient for most methods of x-ray spectral analysis. However, the real luminosity of the x-ray source produced by the interaction of high-power laser pulses with solid targets is an important parameter, which, in particular, gives an understanding for the distribution of the primary energy input along different excitation channels.

Semiconductor detectors for hot plasma diagnostics

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The paper describes the results on development and research characteristics of the semiconductor x-ray detectors for diagnostics of hot plasma parameters on high-power laser and electro-physical facilities. Prototypes of fast Si pin-diodes and GaAs Schottky diodes for detection of x-ray pulse shape in the energy range of 0.5–30 keV have been developed at VNIIA. Prototypes of highly sensitive single-crystal CdTe photoresistor have been developed to measure the energy yield of pulsed and continuous running x-ray systems. Detectors may be operated either as an individual device or as a part of multichannel systems (spectrometers) under the atmospheric pressure or below 1×10^{-4} Torr. The paper contains the research results for basic characteristics of detectors such as dark current, peak linear pulsed current, time resolution and quantum efficiency.

Investigation of the elemental composition of N-doped titanium dioxide thin films by Rutherford backscattering method

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Currently, the Rutherford backscattering (RBS) is one of the most common analytical methods of analysis. The method makes it possible to carry out non-destructive analysis of the elemental composition and structure of the samples in the near-surface region, which makes it indispensable in solving practical problems related to the modification of the properties of solids. The method is based on the irradiation of the sample by a beam of fast ions. Further, energy spectra of ions that have experienced elastic scattering at large angles are recorded. In our work, the subject of the study are coatings of pure titanium oxide and titanium oxide doped with nitrogen (N-TiO₂) on a stainless steel substrate. Coatings were obtained by reactive magnetron sputtering. Deposition modes: the ratio of the partial pressures of the gases $p(\text{O}_2)/p(\text{N}_2)$, the deposition time 180 min, the bias voltage $U_{\text{cm}} = -100$ V. The beam of accelerated helium ions used for the analysis of coatings had an energy $E = 2.035$ MeV. Geometry of the experiment: $\Theta_1 = 30$, $\Theta_2 = 20$, scattering angle $\Theta = 170$. The energy thickness of one channel E in this experiment was 2.06 keV. Elemental analysis and coating thickness analysis were carried out. It is shown, that the samples had a uniform distribution of titanium and oxygen elements and the presence of nitrogen N, and the thickness of the coating was consistent with the ellipsometric method of determining the thickness.

Investigation of zirconia plasma electrolytic oxidation coatings by nuclear backscattering spectrometry

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Zirconia coatings obtained by plasma electrolytic oxidation (PEO) demonstrate low thermal conductivity and high adhesion that makes them promising for use as thermal barrier layers. Low thermal conductivity of coatings can be associated with their layered structure. In this work the layer-by-layer structure of zirconia PEO coatings with a thickness of up to 80 μm formed in silicate-alkaline and silicate-hypophosphite electrolytes was investigated. The study of the composition distribution over the coating thickness was carried out by proton nuclear backscattering spectrometry (NBS) using a 120-centimeter cyclotron. The proton-beam energy was 7.4 MeV. A comparison of the geometric and mass thicknesses determined by the NBS was allowed to estimate the total porosity of the coatings. The coating structure was studied by scanning electron microscopy and x-ray diffraction. NBS data analysis showed that the thickness of the upper layer with an increased silicon content is several times higher for the PEO coating obtained in the silicate-hypophosphite electrolyte. The main middle layer of the PEO coating obtained in the silicate-hypophosphite electrolyte is homogeneous in composition, and for the PEO coating obtained in the silicate-alkaline electrolyte, the amount of oxygen decreases substantially with increasing depth, which indicates the presence of a thicker transition layer. The study was supported by grant from the President of the Russian Federation No. MK-524.2017.8.

Longitudinal electric field: From Maxwell equation to non-locality in time

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In this work, we use the classical electrodynamics to show that the Lorenz gauge can be incompatible with some particular solutions of the d'Alembert equations for electromagnetic potentials. In its turn, the d'Alembert equations for the electromagnetic potentials are the result of application of the Lorenz gauge to general equations for the potentials [1, 2]. The last ones is the straightforward consequence of Maxwell equations. Since the d'Alembert equations and the electromagnetic potentials are necessary for quantum electrodynamics formulation, one should oblige to satisfy these equations also in classical case. The solution of the d'Alembert equations, which modifies longitudinal electric field is found. The requirement of this modification can be justified from the necessity to satisfy the physical condition of impossibility of instantaneous transferring of interaction in space. The comparison with other particular solutions of the d'Alembert equations is discussed.

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Dark matter creation in the antimatter–antimatter collisions

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Dark matter (DM)–dark energy (DE) could be created by N dark standard model (SM) Universes or the shadow mirror Universe by Okun and Pomeranchuk. But if the SM Universes form the spatially ordered chain of very thin, flat parallel 3D-waveguides, periodically placed in the Euclidean 4D-space, then (a) the united—waveguided special relativity–wave quantum mechanics–Newtonian gravity and equivalence principle co-emerge with (b) the CPT and $\pm M_{\text{gr}}$ symmetry (matter–antimatter antigravity) between the SM-coupled—co-visible adjacent $2n/(2n + 1)$ Universes as the repulsive DE nature by zero cosmological constant, (c) the SM-decoupled—mutually dark, attractive $2n/(2n + 2)$ Universes as the DM and DE–DM-finetuning nature, (d) the repulsive $2n/(2n + 1)$ DM–Dark Antimatter SM-Universes, shaping our composite, gravitationally neutral large-scale Universe [1–3]. Our ordered SM-composite concept predicts: (i) The matter/antimatter antigravity (in the antihydrogen CERN-test 2018; (ii) Only antimatter able detect cosmic DM-particles (dark electrons, dark protons, etc) as the only DM–matter SM-mediator; (iii) only antimatter–antimatter (e^+/e^+ , p^-/p^- , e^+/p^-) collisions, never done, can create (test) these N -natural DM-particles, even in low energy colliders [4].

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Resonance reflection of light from a $\nu = 1/3$ Laughlin liquid

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Resonance reflection of light from a two-dimensional electron system in a strong magnetic field has been investigated in an ultra-quantum limit. A line associated with the formation of a Laughlin liquid in the electron system has been discovered. Similar features have been observed in neither photoluminescence nor resonance Rayleigh scattering spectra. The new line appears in the symmetric electron system at zero momentum transfer in the translationally invariant system. The new line is blue shifted. The magnitude of the shift can be interpreted as a transport Coulomb gap required for the creation of a neutral defect in an incompressible Laughlin liquid. Reflection spectrum consists of two main lines. The intensity of one line is weakly sensitive to the temperature of the electron system. The other, high-energy line disappears already at a temperature of 1.6 K. The low-energy line corresponds to the optical transition to the upper empty spin sublevel of the zeroth Landau level of electrons from the zeroth Landau level of heavy holes. In the photoluminescence spectra, on the contrary, the transitions from the lower occupied spin sublevel of electrons are dominated. The oscillator strength of the optical transition is redistributed between two lines in the region of the formation of the Laughlin liquid ($1/3$): the low-energy line coinciding with photoluminescence of electrons on the upper Landau spin sublevel and the high energy line blue-shifted by 0.7 meV. The observed blue shift can be attributed to the creation of three negatively charged Laughlin quasiparticles and quasi-holes neutralizing them.

Influence of radiation effect on mobility of edge dislocations in iron–chromium crystallites

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A molecular dynamics study of the radiation influence on the mobility of edge dislocations in iron–chromium crystallites has been carried out. The simulated crystallite had the form of a parallelepiped. In two directions, periodic boundary conditions were used, in the third direction a shear load was applied to opposite faces of the crystallite. The temperature of the simulated crystallite was 300 K. Interatomic interactions were described on the base of the embedded atom method. Used potentials allowed describing with high accuracy many mechanical and physical properties which are very important for the simulations of metal behavior under radiation exposure. The threshold shear stresses are calculated, which cause displacement of edge dislocations in the Fe–Cr alloys both with an ideal structure and with different concentration of point defects. The features of the propagation of edge dislocations through radiation-damaged regions in an elastically stressed crystallite are studied. To form the radiation damage in the crystallite, cascades of atomic displacements generated by primary-knocked out atoms with different energies were generated. The effect of variable shear loading on the mobility of edge dislocations in iron–chromium alloys is studied. The work was performed with financial support of the Russian Foundation for Basic Research, grant No. 16-08-00120.

Exact solutions for the blade-like surface configurations of a conducting liquid in an external electric field

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The problem on equilibrium configurations of the free surface of conductive capillary fluid in an external electric field is considered in a two-dimensional plane-symmetric formulation. It was previously proved that, in the limiting case of an infinite interelectrode distance, equilibrium configurations providing the unlimited local amplification of the electric field do not exist: all solutions to the problem have no physical meaning (they are self-intersecting) [1].

In the present work, we study the case of a finite interelectrode distance (the distance between the liquid surface and the flat electrode is comparable with the curvature radius of a deformed surface). Using the approaches proposed in [2,3], exact solutions of this problem are constructed. According to these solutions, the surface takes the shape of a blade. Such configurations ensure unlimited local amplification of the electric field: its strength is maximal at the edge of the blade and decreases to zero at the periphery. For a given potential difference between the liquid surface and the flat electrode, the threshold values of (i) the electric field strength at the edge of the blade and (ii) the distance from the edge to the electrode are found. These values confine the domain of existence of the solutions.

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Hydrodynamic characteristics of weakly conductive liquid media in the high nonuniform electrical field

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The investigations were carried out in the interelectrode gap of the “wire above the plane” system of high-voltage electrodes with a constant applied voltage in the range from 0.5 to 5.0 kV. A system of macroscopic differential equations with corresponding boundary conditions was derived and solved. An approximate analytical solution is obtained using known hydrodynamic solutions for the jet flows of a viscous fluid and a more accurate numerical solution by the MacCormack method, taking into account the effect of the space charge and its convective motion. Based on the results of numerical calculations, the velocities maximums of eddy flows from a thin high-voltage wire, observed in the experiments, are determined. The order of these maximums reaches several cm/sec. When the voltage was increased to 4 kV, vortices near the plane electrode were numerically obtained. It is analytically shown that such vortices are an electrohydrodynamic analog of the Heal vortices known in hydrodynamics.

Electromagnetic information technology for human body investigation

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There is no doubt that between the most important achievements in modern medical diagnostics methods we could point the different types of computer tomography for human body: x-ray tomography, magnetic resonance imaging (MRI) tomography, positron emission tomography (PET), gamma-ray tomography etc. These methods allow doctor to see the position and pathologies of internal organs without opening the body. Unfortunately, installations for computer tomography methods mentioned above are quite cumbersome and expensive. Also all of them are rather invasive. The medical treatment by these types of computer tomography is quite long: about half an hour per patient, so their capacity is quite low. During last 20 years, IRE RAS develops a new noninvasive method of computer tomography: electric impedance computer tomography (EICT). It is very important to see the functioning of the organs since the malfunction of organs usually (excluding accidents etc) occurs much earlier than pathological changes appear. So revealing patients, whose homeostasis is just about to go outside of its dynamic stability range, gives possibility to return them to norm by mobilization of internal reserves of their organism. It is very important also for monitoring of the results for all kinds of medical treatment in real time to have possibility to correct the treatment course. One of such methods based on remote radiophysical sensing of human body also was suggested by IRE RAS in the beginning of 80th. In the report the description of these new methods will be given and examples of medical diagnostics will be presented.

Remote decapsulation of liposomal capsules by ultrashort electric pulses

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Further progress in biotechnology and biomedicine depends on the creation of novel functional biocompatible and bioactive materials, efficient systems for capsulation and targeted delivery of various functional active compounds. The success in the directions is determined by solution of correlated physical, chemical, biological and nanotechnological tasks and becomes now challenging interdisciplinary problem.

The main questions that have to be solved are the following: (i) How the drug could be capsulated by the carrier and then delivered to definite local area? (ii) How the drug could be delivered and removed from the carrier by a controlled way? (iii) How to decrease potential toxicity of the used materials to minimize their possible negative effects on the organism?

The authors make efforts to develop new prospective system for capsulation and controlled targeted delivery of various compounds in aqueous media based on the colloid nanocomposite vesicles and capsules representing hybrid constructions formed by polymers (including biopolymers and inter-polyelectrolyte complexes), lipids and amphiphiles, inorganic nanoparticles and other functional components. The electric pulses effects on the nanocomposite capsules and remote non-thermal activation of capsules have been studied.

Obtained results confirm the possibility to form hybrid nanocomposite magnetic vesicles and capsules composed of lipids, polymers and nanoparticles whose spatial localization, structure and permeability could be changed remotely by a controllable way through corresponding electromagnetic pulses.

Acceleration of metallic flyers on the Angara-5-1 installation

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Loading of the sample by magnetic field allows to study the dynamic characteristics of substances at sub-microsecond processes. At the Angara-5-1 installation, the megabar pressure is generated by the magnetic field produced by the current with linear density of 5 MA/cm. It was obtained velocity up to 10 km/s during the previous experimental investigations with duralumin flyer with a thickness of 1 mm. The present report contains the results of the experiment to acceleration of flyers made from other metals, such as copper and titanium. The numerical simulation was carried out to estimate the parameters of the flyer made from these metals at the action on it the current with a linear density of ≈ 4.5 MA/cm. The time dependencies of the velocity for different layers of flyers, and their offset against the initial position, and the distribution of the temperature, density, pressure and current density in different time over its thickness were obtained. A comparison of the simulation results and experimental data is presented.

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Dynamics of implosion of wire array on deuterated cylinder at the Angara-5-1 facility

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The implosion of wire array on the internal deuterated cylinder was investigated at the Angara-5-1 facility (3.5 MA, 100 ns). Arrays of various configurations with diameter of 12 and 20 mm were made on the basis of aluminum wires and graphite fibers with a diameter of 15 and 7 μm . Also the mixed arrays consisting of aluminum wires and nylon wires with a diameter of 25 μm and arrays from nylon fibers with an aluminum covering 1 μm thick were used. The quantity of wires changed from 10 to 30. The internal cylinder was made of deuterated polyethylene with density of 0.09–0.3 g/cm^3 and with a diameter of 1–3 mm. It was established that dynamics of implosion of plasma, formation of the hot spots which are sources of neutrons depends on configuration of load: diameter of arrays, quantity of wires (fiber), diameter and density of the deuterated cylinder. The most efficient compression and high parameters of plasma (compression ratio, temperature), and also the maximum neutron output (2.6×10^{10}) was observed in experiments with the array with a diameter of 12 mm consisting of aluminum wires in which the deuterated cylinder with a diameter of 1 mm was located.

Simulation of primary radiation damage in V and V-4Ti alloy

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In the framework of the molecular dynamics method, simulation of the primary radiation damage in crystallites of bcc V and V-4Ti alloy was carried out. The simulated crystallites had the shape of a cube with edge of 12 nm. Periodic boundary conditions were set in the directions [100], [010] and [001]. The initial temperature of the simulated crystallites was 700 K. The interatomic interaction in V and V-4Ti was described on the base of modern potentials of interatomic interactions [1,2]. These potentials accurately reproduce the energies of formation of point defects, moduli of elasticity, melting point, lattice parameter in the simulated alloy. The impact of the decay particle on the atoms of the simulated crystallites, as a result of which a cascade of atomic displacements was generated, was simulated by assigning a pulse to one of the lattice atoms, the primary knocked out atom. The main characteristics of atomic displacement cascades in simulated crystallites were calculated: the number of defects at different stages of cascade development, the duration of the ballistic and recombination stages of cascade development, and the size of the radiation-damaged region. An analysis of the estimation of the number, types and sizes of the surviving radiation defects in crystallites is given. The results obtained are compared for vanadium and V-4Ti alloy. The work was performed with financial support of the Russian Foundation for Basic Research, grant No. 17-308-50026.

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Multiscale modeling and simulation of nuclear materials

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New technologies of nuclear power technologies are deeply connected with the problems of new materials development. Radiation damage of construction materials of nuclear reactors and nuclear fuels are among the most important research topics for the progress of nuclear power engineering. The complexity of theoretical, mathematical and computational description of these phenomena is rooted in the inherent multiscale nature of radiation damage. Elementary act of this damage is a single atom knock-out off the lattice at timescale of about 10^{-12} s. But the final result is the failure of the reactor, swelling of fuel pellets and other undesirable consequences that reveal themselves during year of reactor exploitation.

The multiscale hierarchy consists of the following major levels:

- Ab initio models of electronic structure usually limited by hundreds of atoms and aimed at the most accurate calculations of basic properties.
- Classical atomistic models of large multi-million systems of atoms that represent the most crucial features of mesoscale structure of materials.
- Rate theories and kinetic approaches that encapsulate information from the atomistic calculations and provide data comparable with experimental observations.

In this report, I describe the recent progress in predictive modeling and simulation of the representative list of nuclear materials. The benchmark tests of the multiscale approach and engineering and scientific deployment of the results are considered as well. The work is supported by the Russian Foundation for Basic Research, grant No. 18-08-01495.

Challenges of high temperature sodium use as coolant in nuclear reactors for hydrogen production

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An important issue defining the future development of clean energy is the involvement of hydrogen into the fuel cycle. Hydrogen is a very attractive element for replacing fossil fuels, although it is not a source but a carrier of energy.

As expected, the demand for hydrogen production will increase dramatically in the near future. Methods are being developed to produce hydrogen by methods of splitting water using thermochemical or electrolysis processes that require a high-temperature heat source. Nuclear reactors of generation IV could serve as high-temperature heat sources are thanks to use of such coolants as gases, liquid metals (sodium, lead), salt melts. The temperature at the outlet from the core in these reactors can reach up to 900–950 °C.

In the present work, study in support of the development of a sodium coolant technology at high temperatures and hydrogen concentrations is presented, as well as discussion of the application of heat-resistant radiation-resistant high-temperature structural materials, ensuring their corrosion resistance at an oxygen content of sodium coolant at 0.1 ppm. Specific estimates were made for the BN-VT reactor of 600 MW.

Heat conduction in superheated binary solutions

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The properties of solutions can differ significantly from the additive values of the properties of their constituent components. With respect to the thermal conductivity of solutions, the key characteristic of heat transfer in the case of high-power heat generation, the following hypothesis is accepted: introduction of a second component into the pure system leads to the appearance of an additional thermal resistance. It was found that an increase in the positive values of excess volume of the solution is accompanied by a decrease in its thermal conductivity. To determine the degree of generality of this hypothesis, experiments were carried out with a class of solutions characterized by negative values of the excess volume. Due to the requests of impulse technologies, measurements are performed, along with the region of stable states, in a wide region of superheated states (with respect to the liquid–vapor equilibrium line) that are inaccessible to traditional methods. Using the method of the temperature plateau, the value of the additional thermal resistance of the solutions: isopropanol with water, ethylene glycol and triethylene glycol, and also an aqueous solution of triethylene glycol was determined. The experiments were carried out at atmospheric pressure and temperatures up to 180 °C. It was found that, contrary to formal extrapolation of the dependence of the thermal conductivity on the excess volume, solutions with a negative excess volume are also characterized by a decrease in the thermal conductivity over the entire range of the concentration change.

The study was partially supported by the Russian Foundation for Basic Research, research project No.16-08-00381 and the comprehensive program of the Ural Branch RAS, research project No.18-2-2-3.

Explosive electron emission and ectons

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In physics, there are several ways to extract electrons from a metal. Generally, electron emission is a process in which individual electrons escape from a metal. This report deals with the phenomenon of occurrence of not individual charged particles but particle bunches (containing up to 10^{10} – 10^{12} particles) within a short time (10^{-9} – 10^{-8} s). These charged particle bunches are formed as a result of microexplosive processes that occur due to high energy concentrated in a microvolume on the cathode surface. We call them ectons. Explosive electron emission (EEE) is the ejection of electrons from the surface of a conductor (cathode) as a result of an explosion of the conductor material in a microscopic volume on the surface. The explosion and the initiation of EEE may occur for various reasons. However, the most conventional mechanism of EEE initiation is the fast heating of cathode microareas by field emission current, whose density may reach 10^9 A/cm² if the electric field is high enough. The report contains information on recently discovered phenomena in EEE physics, such as the effects of shunting and screening, the ring effect, the stroke effect, etc.

Explosive emission processes in thermonuclear facilities and electron–positron colliders

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Explosive electron emission arises at metal surfaces under the action of intense energy flows and high electric fields. The initiation of the emission is accompanied by the transition of the metal from a condensed to a plasma state, which possesses high emissivity making feasible essentially unlimited pulsed electron currents. Explosive electron emission is the basis for the operation of extraordinary pulsed power systems, such as electron accelerators, x-ray generators, lasers, and microwave oscillators. We consider another aspect of explosive emission processes: the cases in which they need to be suppressed. This is in reference to the most important international projects, such as the International Thermonuclear Experimental Reactor (ITER) and the multi-TeV linear electron-positron collider (CLIC). In the first case, explosive electron emission initiated on the first wall and on the divertor is potentially a source of contaminants and impurities in the thermonuclear plasma. In the second case, the plasma produced by explosive electron emission on the surface of the accelerating structure limits the strength of the accelerating electric field. Estimates of the parameters characterizing the initiation and self-sustaining of explosive emission processes under the conditions of operation of ITER and CLIC are presented.

High-energy proton microscopy for extreme state of matter research

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Existing proton radiography facilities, constructed according to the scheme of high-energy proton microscope with image magnification, in USA (pRad at Los Alamos National Laboratory), Russia (PUMA at ITEP) clearly demonstrated the advantages of the high-energy proton radiography method compared to conventional x-ray techniques in the study of solid objects and dense plasma, especially in dynamic experiments. The new proton microscope for an investigation of fast dynamic processes with areal density of targets up to 5 g/cm^2 is under designed on the basis of high-current proton. With this setup, by using of 247 MeV proton beam plan to investigate of solid targets and shock-wave processes in dynamic. Novel high-energy proton microscope called PRIOR will be the key diagnostic instrument for research program of HED@FAIR collaboration at FAIR project. PRIOR prototype, with using of quadrupole lenses on permanent magnets, was designed and commissioned on the synchrotron SIS-18 at GSI in 2014. The spatial resolution of $30 \mu\text{m}$ was achieved in the first experiments at PRIOR setup, with 3.6 GeV proton energy. New version of setup PRIOR-II, with using of electromagnetic quadrupoles, will provide spatial resolution better than $10 \mu\text{m}$. PRIOR-II will work with beam energy 2–5 GeV, which will provide investigate targets with wide range of densities.

Design and modeling of facilities for proton radiography

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Calculation and modeling of ion optics of installation for proton radiography—the tasks which need to be solved not only in procedure of designing of radiographic installation, but also during its regular operation. Calculation and search for the best placing of the magnetic elements on the ion-optical scheme of the projected installation is performed in the COSY Infinity [1] environment, based on the principle of matrix formalism [2]. The created calculation program allows to optimize the installation parameters such as fields and mutual arrangement of magnetic elements, monitoring the quality of the beam focusing in the key planes of the installation. The calculations are checked using the Monte-Carlo simulation of a proton microscope in the GEANT4 environment. For this purpose, a set of tests and test targets are used to evaluate the resolution, contrast, and dynamic range of the installation. The results of calculations for the 247 MeV facility [3] on the linear accelerator INR (Russia, Troitsk) are demonstrated, which is planned to be created using the technical base of the PUMA installation (ITEP, Moscow) [4]. And PRIOR-II installations (proton energy 2–5 GeV) [2]. The calculations of the PRIOR-II facility were carried out on the basis of the information obtained from the PRIOR-Proton Microscope for FAIR TDR [2], for the beam energy of 4 GeV.

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Numerical simulation of proton-radiography experiments at PRIOR-II with Geant4

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The high-energy proton radiography in the investigations of dense dynamic target provides greater penetration depth, spatial resolution, density resolution and dynamic range than conventional x-ray methods [1,2]. The high-energy proton microscopy facilities PRIOR-II (2–5 GeV beam energy) [2] will be one of the key diagnostic tool for high-energy-density-physics experiments at FAIR project. Using this facility, the spatial resolution of proton-radiographic image better than 10 μm can be reached. The ion optics of facility [3] was designed according to the schemes of proton microscopes with magnifying an image of objects. In this work, using Geant4 code, the full-scale Monte-Carlo numerical simulation of future proton radiography experiments was performed. The virtual model [4] of PRIOR-II facility was developed based on ion optical data described at PRIOR proton microscope for FAIR TDR [3] with energy of the beam 4 GeV. The full-scale numerical simulation for PRIOR-II was performed for static objects (Cu, polymethylmethacrylate step wedges) and static models of dynamic process, such as electrical explosion of Ta-wire in water and investigation of compressibility of Ce. Developed model can be used for the future proton-radiography experiments at PRIOR-II facility at FAIR project.

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Formation of submicron thickness films under processing graphite by proton beam

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Modification of graphite surface under irradiation by beam of protons with energy 50 keV was studied. Protons flux was equal 4×10^{15} and $2 \times 10^{16} \text{ cm}^{-2}$. It was established that under the proton action the sample surface was converted into a periodic structure in the form of ridges, located in increments of less than $1 \mu\text{m}$. Increase in radiation dose led to a more intensive growth of discovered structures. The transparent thin films were detected on the graphite surface with help of scan electronic microscope. The action of the arc discharge on the modified surface of graphite was described.

A device for measuring spectra of neutron radiation

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The developed device for measurement of energy-angular distributions of neutron radiation for experimental research of technical protective characteristics in samples of special technique. During the development of this device it is based on the design of “all-wave” counter pro-posed by Hanson and Mac-Kiben. The component parts of the device are: collimator neutron radiation; boron filter that absorbs thermal neutrons from neutron radiation incident on the lateral surface of the counter; the measuring unit of cylindrical shape from a material containing hydrogen (for example, paraffin or Plexiglas), inside which are placed activation detectors in a special insert. The neutron detectors in the form of plates Dy^{163} placed in pairs in the cadmium covers and without covers along the axis of the measuring unit. The difference in their readings allows you to determine the fluence of thermal neutrons to the corresponding points of the measuring unit. The distribution of thermal neutrons $S(E, L)$ along the axis of the measuring unit, where L is the distance from its end surface depends from the neutron energy E , incident on end surface. This allows to assess the energy distribution $f(E)$ of neutrons by solving the integral equation.

Transmission of high frequency analog waveform at first transmission window and streak camera detection

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When the high power laser-beam facilities are used for analysis, the diagnostics of hot plasma is made through detection of pulses from associated emission (optic, x-ray, neutron, etc) applying various detecting systems. Due to nanosecond and subnanosecond duration of processes under investigation, harsh environment it is crucial to transmit the analog signals from detectors to registrators, which are usually several tens or hundreds of meters distant from each other, without loss and distortion. The conventional transmission systems based on coaxial cables prevent from transmitting the signals of required quality. The paper describes the fiber optic-based analog transmission system with the external modulation at first transmission window and the streak camera detection.

Microwave action on the synthesis and stability of selenium nanostructures

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Nanoselenium still remains very popular subject of investigations nowadays thanks to the great number of applications. As for recent advances in this field for example it is creation of composites of high-molecular substances and nanoselenium for high energy accumulator batteries with cycling stability and large capacity, removing of mercury from groundwater with the help of selenium composites. Selenium nanoparticles have wonderful property as essential nutrient supplement from its lower toxicity and ability of gradual release of selenium. Composites of proteins with nanoselenium having antibacterial and anticancer action and long time of storage, rather uniform particle size distribution were successfully obtained. The same problem we dissolve in research of our systems as for properties of the final product of synthesis. We have treated in microwave furnace the mixture of water solutions of polymer, surfactant, electrolytic addition, selenite, sulfurous acid and in some experiments every solution separately before treatment of the mixture. Final product of this procedure was dried polymeric film. It was characterized with electronic and optical microscopy, ultraviolet visible and Raman spectroscopy. Conclusions were made on mechanism of processes and influence of reaction parameters on the properties of final product.

Some new results in one-, two- and three-dimensional discrete-ordinates codes for solving the time-dependent transport problems

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The one- (1D), two- (2D) and three-dimensional (3D) steady-state transport codes ROZ-6.6, KASKAD-S-3.5 and KATRIN-2.5 from CNCSN-2 code system have been successfully extended for solving the time-dependent transport problems by the discrete-ordinates (S_n) method. A new time-dependent codes ROZ-W-3, KASKAD-W-2 and KATRIN-W-1 solve the time-dependent multigroup transport equation for neutrons, photons and charged particles in 1D, 2D and 3D geometries, respectively. In the present work main features of time-dependents S_n codes are described: the second-order of accuracy adaptive weighted diamond difference (AWDD) scheme for temporal, spatial and angular variables in transport equation; the consistent P1 Synthetic Acceleration (P1SA) scheme for acceleration of inner iterations convergence; the special algorithm for calculation of the unscattered flux from pulsed sources. The K -th order of accuracy semiexplicit K -step scheme for the spatial discretization is discussed. The new results of using of 1D, 2D, 3D S_n codes for solving the time-dependent benchmark transport problems are presented.

Modeling of the extreme state of the thermal-protective cover of the rocket technique constructions to optimize their composition

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The roentgen radiation of the high-altitude nuclear explosion is the main affecting factor for aircraft devices in the upper layers of atmosphere and space [1]. One of the possible harmful factors for the rocket technique is the radiation of the continuous laser as well [2]. In the present work we suggest the computational-experimental approach to choose and optimize the element composition of the perspective multifunctional protective cover of the rocket technique from the roentgen and laser radiations.

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New method of evaluation of thermal characteristics of complex heat shield assemblies under extremely high energy densities and nearly one-dimensional conditions

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One of the possible ways of constructing of an advance thermal protection materials subjected to extreme heat fluxes is still based on the use of various kinds of the carbon-carbon composite materials. The aim of the present study is to develop a suitable experimental procedure where a small fragment of the relatively thick heat shield is exposed to the required extreme heat flux during several tens of seconds while keeping almost one-dimensional conditions. The needed heat flux is produced by the cw-laser, which power can be regulated according to the arbitrary function. The fragment of the carbon-carbon composite of cylindrical shape was surrounded by zirconia concrete used as a high-temperature thermal insulation. The free front face of the sample is heated by a high power laser, while the temperature in the center of the front face is measured by the high-speed pyrometer. The temperature of the rear face of the cylindrical sample and its lateral face is measured by a few thermocouples inserted through the thermal insulation. The obtained results confirmed that the proposed method can be successfully used for evaluation of the complex high-temperature heat protective assemblies.

Entanglement network evolution with disentanglement dynamic during deformation of carbon-nanotube-reinforced polyethylene nanocomposite

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In recent decades glassy polymers are interesting for material science due to their unique mechanical properties such as expansivity or viscoelastic. Of the great interest is the establishment of the behavior of glassy polymers on adding carbon nanotubes to their molecular structure. Molecular dynamics (MD) gives the opportunity to build this model with great predictable capabilities. In this work we introduce the results of MD simulation of glassy polymer with single-walled carbon nanotubes under tensile deformation. Primitive path (PP) analysis was used to study the entanglement structure evolution and disentanglement dynamic of polymer chains under the tensile deformation [1]. Besides the mechanical properties of the material attention is given to the accuracy of MD computation using the power of high-performance supercomputer.

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Carbon additive structure influence on electrochemical double-layer capacitor high-current behavior

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Electrochemical double-layer capacitors (EDLC) are widely used as power sources for peak load or peak generation leveling in transport [1] and stationary applications [2]. Carbon nanotubes (CNT) as alternative to carbon blacks as conductive additive for electrodes are good possibility to improve high current operation both for accumulators and EDLC. In [3] possibility of capacity increase in case of CNT application in EDLC was shown. Two types of CNT, high quality TuballTM from OCSiAl (Novosibirsk, Russia) and TaunitTM from NanoTechCenter LLC (Tambov, Russia) with different additive loads were used as carbon additives for electrodes, prepared as described in [3]. Taunit structure is close more to nanofibres than to single-walled nanotubes (as Tuball material is) but this additive is less expensive than Tuball and EDLC cost is also important parameter for final customer. Also electrode samples with Vulcan XC72R carbon black were prepared for reference measurements. All electrode samples were tested in galvanostatic charge-discharge mode at different current levels in laboratory-scale EDLC cell, characterized by scanning electron microscopy. Obtained results showed improved high-current operation for CNT-containing electrodes, especially in case of Tuball.

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Pyro-polymeric cathode catalysts for air-aluminum fuel cells synthesis and research

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Air-aluminum fuel cells (AA FC) consist of Al anode, alkaline or salt electrolyte and composite carbon-polymer cathode. Aluminum corrosion in electrolyte and oxygen reduction reaction (ORR) on cathode are current-forming reactions for AA FC. One of the advantages of such elements is the high specific energy density [1]. Currently, the main research and development activity in the field of AA FC has the goal of creating backup and portable power sources for military applications, as well as energy sources for electric vehicles. Sluggish cathode reaction is the main difficulty on the way to high-power AA FC, so role of cheap but inexpensive catalyst and well-organized cathode electrode structure is crucial for progress in practical AA FC applications. Platinum nanoparticles are known to be the best catalyst for ORR [2]. But precious metals consumption must be reduced for successive commercialization. In this paper synthesis and test in laboratory-scale AA FC of a pyro-polymer of cobalt tetra (p-methoxyphenyl) porphyrin (PP TMPPS) is described. Cathodes with activated carbon were also tested as reference samples.

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Effect of carbon cathode morphology on the kinetics of the heterogenous processes in Li-air batteries

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The current work is devoted to the investigation by the method of classical molecular dynamics of the influence of carbon surface morphology on the cathode–solvent interface structure near the following model cathodes: graphene plane, nanotube, single- and multi-layer graphene edges. Two types of solvents were examined. Acetonitrile (ACN) is a low donor number (DN) solvent (DN = 14) and dimethyl sulfoxide (DMSO) is a high-DN solvent (DN = 30). It was found that the morphology of the carbon surface qualitatively influences the cathode–solvent interface structure and, as a result, the distribution of the main reactants (Li^+ and O_2) of the oxygen reduction reaction [1, 2]. The free energy profiles for Li^+ and O_2 near the model cathodes were found. It was shown that the adsorption barrier of O_2 molecules decreases in the order graphene plane \rightarrow nanotube \rightarrow graphene edge. This can explain the increased formation of the reaction products at graphene edges, observed in the experiments. Also the local minimum, which corresponds to the position of adsorbed Li^+ ions, is not observed in DMSO. This effect is associated with the formation of a stable solvent shell around lithium ions in high-DN solvents.

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The influence of segregation effect on defect distribution between volume and surface in α -Al₂O₃

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The impurities existence in the crystal and their distribution between volume and surface influence significantly on different physical properties of the material: oxidation rate, electrical conductivity, optical transparency, etc. It was shown that this influence is linked with segregation effect. Thus, understanding what impurities and in what form mainly accumulate in the interphase boundary is necessary step in order to predict the influence of impurities on material properties.

Molecular dynamics method was used for the calculations. Ionic model of aluminium oxide was applied.

The model was proposed to describe the equilibrium distribution of impurities between the volume and free surface of aluminium oxide, taking into account the clustering of defects due to electrostatic interactions; the model is validated.

The segregation effect in α -Al₂O₃ doped with magnesium was studied. It was shown that Mg has pronounced tendency to segregation and on surface it is predominantly in the form of atoms, replacing the ions Al³⁺ in the lattice.

Since the defect Mg_{Al}^{surf} (Mg ions, replacing the Al ions on the surface) has the highest concentration and effective charge in the lattice -1 , the mechanism of compensation the charge should exist for preservation of electric neutrality of a crystal. In this work was shown that depending on the level of impurity and temperature, different mechanism of charge compensation can exist.

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Molecular dynamics simulation of solvent and ion radius influence on the structure of ion solvation shell and ion diffusion

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The impact of solvent and metal cation radius on the cation behavior was studied by molecular dynamics simulation, which plays a crucial role in the chemical reactions of metal-air batteries. The investigation of solvent effect was carried out for lithium ion by using three solvents: acetonitrile (ACN), 1,2-dimethoxyethane (DME), dimethyl sulfoxide (DMSO) with various donor numbers (DN = 14, 20, 30 respectively). The simulation analysis shows a correlation between the residence time of solvent molecules in the ion solvation shell and the solvent donor number, residence time reaches 100 times larger value in DMSO than in ACN. In DMSO and DME the lithium cation diffuses with its solvation shell as a whole, while in ACN it diffuses as a “bare” ion due to weak solvation. However, the variation of the radius in the range (0.5–2 Å) shows a significant dependence of the ion radius on the ion behavior in the solvent. We found out that there is a sharp maximum of the residence time at a radius of 0.7 Å in ACN. It reaches 10 times larger value at this radius than at lithium ion radius (1 Å). On the contrary, ion diffusion coefficient has a minimum at this radius. All computations were carried out using the clusters of Joint Supercomputer Center of RAS (MVS-100K, MVS-10P). The work was supported by RSF grant No. 14-50-00124.

Efficiency of various schemes of torrefaction reactors and energy technology complexes based on them

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In recent years, interest in the development of solid biofuel production technologies has been growing steadily throughout the world. One of these technologies is based on the use of the process of low-temperature pyrolysis (torrefaction), which allows to significantly increase the consumer characteristics of solid biofuel due to the increase in specific energy content and improvement of hydrophobic properties. The energy efficiency of the technology of torrefaction essentially depends on the method of supplying heat to the processed raw materials: through the wall of the reactor or by direct contact of the biomass with a heat transfer gas. As a heat transfer agent, both volatile products of torrefaction [1] and exhaust gases of a gas piston engine can be used [2]. For the utilization of volatile products of torrefaction, which are hazardous to the environment, thermal methods are commonly used. Thus, depending on the method of heating processed raw materials, the final products of the technological process are: solid biofuel with improved consumer characteristics, thermal and electric energy. The paper analyzes the advantages and disadvantages of each possible variant of the organization of technological process. Corresponding schematic diagrams for its implementation are presented, the results of comparison of different kinds of torrefaction reactors and energy technology complexes on their basis are presented.

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Usability of exothermic reactions heat during torrefaction for process energy efficiency increasing

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A promising technology for pre-conditioning of solid hydrocarbon fuel from plant biomass is torrefaction. Torrefaction is a biofuel processing method, consisting in heating in an oxygen-free environment up to temperatures in the range of 200–300 °C, followed by holding for certain time.

A significant role in achieving the high quality of the torrefaction process organizing is played by thermal processes accompanying the thermal destruction of the convertible biomass. The endo- and exothermic reactions accompanying biomass torrefaction process can appreciably influence the main operating parameter—the torrefaction temperature. The main organic part components of any plant biomass are hemicellulose, cellulose and lignin. Moreover, the decomposition of hemicellulose and lignin shows a pronounced exothermic character, unlike cellulose, the destruction of which is accompanied by the occurrence of endothermic reactions. Taking into account exothermic reactions heat when designing an industrial torrefaction plant can conduce process thermal efficiency increasing. The initial stage in exothermic self-heating process study during torrefaction process was an experimental prototype. This experimental plant is a complex where combustion products of a gas reciprocating engine are used as a coolant.

As part of this research was experiment series on a pilot plant in order to study possible ways of thermal effects rational using. The implementation of the results obtained in experimental studies will reduce external sources heat consumption during the torrefaction process, which will greatly enhance the process energy efficiency.

The influence of various factors on the biomass torrefication

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To use local fuel and energy resources: peat, wood and agricultural waste, including various types of waste products in the fuel and energy balance, low-temperature pyrolysis is used—torrefication (from the English word torrefy, meaning “burn, dry”), which improves qualitatively consumer properties of biomass as fuel—the calorific value and hydrophobicity increase.

Studies of low-temperature pyrolysis of biomass are being carried out at the JIHT RAS.

For the purpose of multifactor analysis and systematization of experimental data obtained during experiments on biomass trimming in the JIHT RAS, a database with a visual interface was developed and allows visualizing the dependences of productivity, operating temperature and other parameters on the power of the GPU, the coolant flow, the type of biomass, etc.

Hydrothermal carbonization of biomass

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Biomass is a renewable energy source, that could be used for reducing a ecological problem such as carbon dioxide emission. In the traditional energy industry about 43% of the carbon dioxide emissions generates during the process of burning coal. In the European Union the coal is replaced by bio-coal to reduce carbon dioxide emissions. Bio-coal is an alternative to wood pellets. The benefits of bio-coal is better transport characteristics and the possibility of using in co-combustion with coal. Hydrothermal carbonization (HTC) is one of the modern methods for obtaining bio-coal. HTC or “cold charring” is a process of coal production from the biomass of different origin. One of the main advantages of hydrothermal carbonization is the possibility of processing biomass of high humidity (up to 80%). The main product of the reaction is a bio-coal which is similar to anthracite in physical characteristics. The obtained carbon can be dewatered mechanically due to its hydrophobic properties. Hydrothermal carbonization proceeds at about 200 °C in aerobic conditions and in the presence of water. The pressure is corresponding to saturated steam one at the temperature used and water is in subcritical conditions. At the Joint Institute for High Temperatures RAS, researching of process of the hydrothermal carbonization of biomass is started. Peat from deposits Mayak of the Novgorod region is the main raw material for study. The influence of temperature on the process of peat processing during the hydrothermal carbonization was studied. It was found that the temperature increase affects on the thermophysical characteristics bio-coal.

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

The influence of oxygen on the low-temperature pyrolysis of biomass

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Improving consumer properties of solid biofuels (decrease hygroscopicity, increase calorific value) achieved in the process of torrefaction—these are processes of low-temperature pyrolysis of biomass—heating of the raw material in an inert gaseous medium to a temperature of 250–270 °C. The installation for studying the processes of low-temperature pyrolysis of biomass was created in the JIHT RAS. A feature of the installation is heated biomass through the exhaust gas of the internal combustion engine (mini-power stations) through the solid granules, the dried biomass (pellets). A series of experiments was conducted to study the effect of oxygen on the process of torrefaction on the installation. The oxygen content in the combustion products varied from 0.5 to 2% in the course of the experiments. Studies have shown that a slight increase in oxygen content by 1% increases the rate of heating of the processed raw materials by 20%. Based on the processed data and the analysis performed, a mathematical model was constructed that takes into account most of the processes and reactions in the reactor of the torrefaction, and a numerical calculation program was developed. The results of calculations and experimental studies are presented in the research work.

Experimental investigations of the two-stage pyrolytic processing of wood biomass and the pyrolysis products properties distribution in a cylindrical retort

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The results of investigations of the character of the distribution of the temperature field in the wood biomass briquette subjected to pyrolytic processing in a cylindrical retort imitating a pyrolysis section of a two-stage biomass processing plant into synthesis gas are experimentally studied.

The dependence of the products characteristics of two-stage pyrolytic processing of wood biomass on the pyrolysis temperature was studied. This, together with the obtained temperature dependence of the briquettes from the heating time, allowed the properties of the biomass processing products to be fully described as applied to calculating the pyrolysis section of a two-stage biomass processing plant into synthesis gas [1].

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

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Dynamics of heating of biomass at the initial stage of low temperature pyrolysis process

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Getting to high-quality solid fuels from woodworking industry processing waste and agricultural waste by thermal treatment (torrefaction of biomass) is an important task in the light of solving energy and environmental problems. To study processes of low-temperature pyrolysis in JIHT RAS an experimental setup of torrefaction of biomass (in the form of pellets). Exhaust gases of gas-piston power station, which is working by stoichiometric composition of blends “natural gas–air” with low oxygen concentrations (until 0.5% by volume), is used as heating transfer for the biomass. As processed biomass–wood pellets from different wood species. On the basis of experimental data created a mathematical model describing the thermal processes of low-temperature pyrolysis of wood pellets. The results of calculations are presented in comparison with experimental data. The developed mathematical model allows determining the optimal operating modes of the installation with the aim of improving the energy efficiency of the torrefaction process.

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

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Sewage sludge refers to secondary types of biomass formed as a result of different treatment degrees of primary biomass. One of the main differences of this waste type is the presence in composition of such pollutants as heavy metals. Also a much larger amount of sulfur (more than 1%) is observed in their composition in comparison with types of primary biomass. In this paper, the study results of the pyrolytic processing condition effect (up to 800 °C) on the behavior of heavy metals and sulfur in sewage sludge composition are presented. Concentration of heavy metal and sulfur, solubility in neutral and acid media of heavy metals in the composition of the initial sewage sludge and pyrolysis solid residue are determined. The class of hazard of the pyrolysis solid residue at its disposal is calculated. A method of pyrolysis gas cleaning from sulfur compounds is proposed.

Daily clearness index distributions for ground-based and satellite data

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The major problem of long-term ground-based actinometrical observation usage for solar power units simulation is an insufficient number of actinometrical stations, so an interpolation of actinometrical data yielding necessary accuracy is impossible. The problem was solved in recent decades by numerical simulation and data reconstruction techniques using the results of satellite observation. NASA POWER [1] and CM SAF [2] databases have been constructed based on such data reconstruction. The problems surrounding “satellite data” accuracy in comparison with ground-based observation data are of particular interest. The accuracy evaluation was made by cumulative distribution construction of daily clearness index [3]. The distributions are the base of design methods of estimation of long-term performance of solar power units. Our calculations used surface data from 1261 meteorological stations from World Radiation Data Centre [4], information from NASA POWER and CM SAF. The reasonably good agreement between cumulative distribution curves; this makes it possible to use NASA POWER and CM SAF data in simulations of solar power systems. It has been also shown that calculated cumulative distributions of clearness index are closely fitted by equation suggested earlier by authors, so this functional dependency is universal in quality.

This work is supported by the Russian Science Foundation under grant 16-19-10659.

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Cristallyne and tandem-type thin-film silicon photovoltaic modules comparative tests in Moscow climate conditions

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In 2005–2010, thin film photovoltaic (PV) technologies were quite popular due to relatively low modules costs and low need in silicon or other materials. Amorphous silicon (a-Si) thin films are well known as PV active material with wider light absorption spectrum part than for crystalline silicon (c-Si) which allows better module operation in case of diffuse radiation [1]. Low PV energy conversion efficiency for crystalline ones is a main drawback of such modules. It is also known, that thin film modules have much lower temperature power coefficient, which makes their operation more reliable at hot weather. Nowadays fast progress in crystalline silicon PV technologies led to lower cost for crystalline modules and made thin film technologies less competitive. In JIHT RAS comparative field tests for crystalline and thin film modules were conducted in 2015–2016, using small autonomous power units as a test bed. Experiments showed, that copper indium gallium selenide module has very close to microcrystalline specific energy production, and a-Si tandem module had even higher productivity then multicrystalline one for the whole test period. So even now the best thin film modules can be competitive with the most widespread muticrystalline modules in projects where power plant area is not crucial.

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4. Physics of Low Temperature Plasma

Properties of ultracold Rydberg gas and plasma

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We present a new technique for investigating of ultracold light atoms by using two-photon coherent excitation of the Rydberg states. The influence of the electric field on the shape of the transition line is taken into account, as a result of mixing the close allowed and forbidden levels. We suggest a new nondestructive method for measuring the atomic temperature in a working magneto-optical trap using two-photon spectroscopy with variable directions of probe beams. The work was supported by the Russian Science Foundation (grant No. 14-50-00124).

Diffusion coefficients of charged particles of ultracold in a magnetic field

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The diffusion coefficients for electrons and protons of an ultracold plasma were calculated for the first time by the molecular dynamics method as a function of the nonideality parameter and the value of the magnetic field induction. Earlier, we calculated the diffusion coefficients without a magnetic field and obtained good agreement with experiment. In this regard, we believe that the numerical simulation carried out by us actually reproduces the physical picture of the evolution of ultracold plasma. So, the results of the presence of a magnetic field are also reliable, although they have not yet been experimentally confirmed. It is important to note here that, in contrast to a low-temperature plasma, a strong magnetic field affecting the transport coefficients in an ultracold plasma is a field with induction from 1000 G to several T.

A model of a system of charged particles consisting of electrons and protons interacting according to the Coulomb's law without any limitations at large or small distances is considered. Density of particles varied from 10^{10} to 10^{12} cm⁻³; the temperature of the electrons is from 8 to 100 K, the temperature of the ions is from 1 to 10 K; induction of the magnetic field from 0 to 5 T. Comparison with available analytical expressions is made. The work was supported by the Russian Science Foundation (grant No. 14-50-00124).

Temperature measurement of light atoms by using two-photon resonances

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We present a new non-destructive experimental technique for measuring temperature of ultracold light atoms by using two-photon coherent excitation to the rydberg states [1]. Two-photon resonance are measured by the method of decay resonance fluorescence of atoms in magneto-optical trap. Atomic cloud excited to the rydberg states counter- and co-propagating beam configuration. Then by using convolution of Lorentzian and Gaussian fit we calculate temperature of atomic cloud. This work was supported by the Russian Science Foundation (grant No. 17-72-10285).

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The vacuum system in experimental setup for laser cooling of calcium atoms

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Our research [1,2] is devoted to the creation and study of ultracold plasma and gas of Rydberg atoms of lithium and calcium. As the first step in the calcium project, we investigated Doppler-free resonances on atomic transition with wavelength 423 nm in high temperature cells with cold windows [3]. As the next step, the vacuum system for our experimental setup has been assembled. The air-cooled Zeeman slower for reduction of the atomic beam velocity was developed and assembled. A vacuum at the level better than 10^{-10} Torr was obtained by using the ion-getter pumps. Before pumping, the vacuum part of setup was degased at 300 °C for one week.

The work was supported by the Presidium of the RAS (Basic Research Program Investigation of Matter in Extreme States headed by V E Fortov).

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Molecular dynamics simulation of electrical current in ultracold strongly coupled plasmas

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The present work is devoted to study of the effect of nonideality of a plasma on its conductivity. As an object of research, an ultracold plasma was chosen. Investigation of the kinetics of ultracold plasma is of considerable interest, since in such plasma kinetic processes are determined exclusively by collisions between charged particles. This distinguishes the ultracold nonideal plasma from a nonideal plasma, obtained, for example, in shock waves, where the conductivity is also affected by collisions of charged particles with neutral ones.

In the present work, the ultracold plasma was simulated by the molecular dynamics method. Within the framework of periodic boundary conditions, classical equations of motion were solved using NVE ensemble. Neutral plasma with electron density $n \sim 10^{10} \text{ cm}^{-3}$ and temperatures $T \sim 1\text{--}100 \text{ K}$ was considered. Electrical field E was included in the equations. The conductivity σ was obtained from occurring current using the expression for the current density $J = \sigma E$.

Calculated conductivity was compared with existing theoretical models and simulation results.

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

Laser radiation interaction with strongly correlated plasma

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The research of transitive layer of explosively driven strongly correlated plasma can be carried out using the technique of inclined probing by polarized electromagnetic waves. To construct the spatial profile of the density of plasma charge carriers, angular dependence of s- and p-polarized reflectivities at several wavelengths can be used [1, 2]. The results of new experiments on reflectivity of polarized light on explosively driven dense xenon plasma are presented. The study of polarized reflectivity properties of plasma was accomplished using laser light of the frequency $\nu_{\text{las}} = 2.83 \times 10^{14} \text{ s}^{-1}$ at incident angles up to $\theta = 60^\circ$. With density $\rho = 2 \text{ g/cm}^3$, pressures $P = 10 \text{ GPa}$ and temperatures up to $T = 3 \times 10^4 \text{ K}$ of the investigated plasma, conditions with strong Coulomb interaction (the nonideality parameter up to $\Gamma = 1.8$) were present.

For determination of the equilibrium properties of explosively driven plasma, appropriate gas dynamics calculations were carried out. The plasma composition was calculated within a chemical picture [3]. The integration of Maxwell equations are based on an interpolation formula for dc conductivity, obtained from a systematic quantum statistical treatment of different limiting cases. Results of the calculations with layer temperature profile and ea-collisions as factor are presented too.

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Shock tubes of non-ideal plasma for proton radiography

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Proton radiography is a promising diagnostic tool for study of matter at extreme conditions. Modern proton radiography systems equipped with special magnetic optics provide high spatial and high temporal resolution of the areal density in dynamic targets. Explosive shock tubes of non-ideal plasma for investigation of thermo-physical properties by proton radiography are described. Proposed experiments includes study of equation of state of shock-compressed non-ideal plasma of argon and xenon.

Coulomb logarithm in nonideal and degenerate plasmas

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In plasma physics and astrophysics, the long-range character of the Coulomb or gravitational interaction leads to the appearance of various kinds of divergent integrals. To eliminate the divergences, the Coulomb logarithm is introduced, the determination of which in the case of a nonideal plasma meets certain difficulties (see, for example, [1, 2] and the literature cited therein).

In this paper, different methods for determining the Coulomb logarithm and different variants for choosing the plasma screening constant and the boundary value of the electron wave vector are considered. To take into account the ion–ion correlations, the Ornstein–Zernike integral equation in the hypernetted chain (HNC) approximation was solved numerically.

The calculated values of the electrical conductivity of a hydrogen plasma are compared with the experimental values measured in a megabar pressure range. It is shown that the Coulomb logarithm values should be much less than one in order to agree with the experimental data. A more accurate determination of the Coulomb logarithm requires special experiments at the gas densities, for which electron scattering by ions predominates over scattering by neutral atoms and molecules (for hydrogen this density region is above 1 g/cm^3).

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The effects of ion density on the ion recombination in dense gases and liquids

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Process of ion recombination in dense gases and liquids is considered with various options for choosing the properties of the medium and the ion itself. The dependence of the ion recombination constant in the gas on Coulomb nonideality is established. But this dependence is absent in liquids. Conditions for the position of regions with different regimes of recombination kinetics are obtained.

The dependence of the rate constant of recombination in dense gases on the parameter of the Coulomb nonideality is investigated. The problems of describing ion recombination in both non-parent and parent gas are considered. The process of resonant charge exchange of ions on molecules of the medium is taken into consideration for ions in parent gases. It is established that, in spite of the existing ideas in the literature [1] that there is no dependence of the recombination rate in the diffusion regime on the parameter of the Coulomb nonideality, this dependence actually remains. This dependence can be interpolated in the range of all values of the nonideality parameter of an exponentially decreasing curve. The steepness of the decrease in the rate constant of recombination with an increase in the nonideality parameter decreases with increasing concentration of the background gas. In case of recombination of ions in liquids such dependence of the rate constants of recombination from Coulomb nonideality are not detected. In addition, the dependence of the recombination rate constant on the mass ratio of recombining ions as well as neutral molecules and ions, is studied.

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Physical mechanisms of plasma medicine

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Plasma inactivation of bacteria is one of the first demonstrations of biomedical applications of plasmas. Discharges of different types were successfully and effectively applied for sterilization of both gram-positive and gram-negative bacteria, as well as spores on surfaces, in air and liquids, and had been described elsewhere. Inactivation efficiency of plasmas was investigated various chemical systems, such as air, nitrogen, oxygen, noble gases. The nature of plasma interactions with bacteria is rather complex, and is clearly different for different conditions, e.g. arc discharge at atmospheric pressure, and low pressure glow discharge. In the framework of newly formed and actively growing field on plasma chemistry, “plasma medicine”, understanding of mechanisms of interaction of atmospheric pressure discharges with living objects becomes extremely important. Plasma generated at atmospheric pressure produces a mix of reactive molecules, charges, electric fields, and radiation. The role of all these components has been widely studied, and it was noticed, that inactivation efficiency highly depends on presence of charged species for room air conditions, but radiation effect is almost always negligible. Previously, some attempts have been made to study the effects of corona discharge on bacteria. For example, in nitrogen atmosphere both positive and negative corona was shown to have relatively low inactivation effect, about 1–2 log reduction in tens of minutes of treatment. In contrast, addition of H_2O_2 into air corona discharge system, leads to about 10^3 times higher efficiency of inactivation (with positive ions being slightly more effective, than negative) compared to H_2O_2 only or corona discharge in Ar. In this study, we attempt to classify different types of species created in discharge plasma and assess their importance in achieving bacterial inactivation and wounds treatment.

Parameters of the high-pressure discharge during its radiative contraction

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Results of determination of the discharge channel parameters in iron plasma in a stage of its maximal contraction are presented. Amplitude of a discharge current was of 500–1500 kA, current rise rate of 5×10^{10} A/s, pressure of surrounding gas—5–7 MPa. Results of intensity measurement for own plasma soft x-ray radiation [1, 2] and registration of radius evolution of current channel of the discharge, received with the help of magnetic probe diagnostics [3,4], confirm a hypothesis about radiative character of the discharge contraction. With the help of the developed system of soft x-ray radiation registration the temperature of the discharge hot zone is determined. The error of measurements does not exceed some electronvolt.

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Analysis of interferograms of small plasma objects taking into account the diffraction effect

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In studies of the prebreakdown processes in a gas [1] it is necessary to ensure the registration of images with high spatial and temporal resolutions. This can be provided by laser probing methods, for example, by interferometric methods.

When analyzing an interferogram, the electron density distribution over the object is reconstructed by using the shifts of the interference fringes. This problem is described by the Helmholtz equation with a variable coefficient. Since the equation has no analytical solution, it is solved by low-accuracy graphical methods or various numerical methods. It should be taken into account that diffraction is also contributing to the interference pattern of the micron-sized objects at the defocusing of the optical system. We used the method of smooth perturbations presented in [2] which allows us to solve the equation in the parabolic approximation.

In this paper, the applicability of the method is tested for the parameters of plasma objects obtained in the study [1]. To increase the accuracy of the method, the requirements for preliminary processing of the phase image are established. In solving a direct problem, the effect of the defocusing scale on the shape and features of the interference fringe is shown; the boundaries of the distinguishability of objects on the interferogram are analysed. When solving the inverse problem using experimental interferograms, the density of plasma objects is restored.

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Investigation of small-scale plasma formations in air discharge

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The early stage of the discharge in air inside highly overvoltage gaps with different electrode geometries was studied by laser methods (simultaneous record of interferograms, shadowgrams and schlieren images). Both 3-channel 9-frame optical registration system with a resolution of $\approx 10\text{--}20 \mu\text{m}$ [1] and 6-channel 18-frame optical registration system with a resolution of $\approx 2 \mu\text{m}$ were used to obtain data on the structure and parameters (electron density gradients) of small plasma formations in the discharge gap. The exposure time of each frame in both systems corresponds to the pulse duration of the probing laser—70 ps at a wavelength of 532 nm.

It was shown that during breakdown the plasma with electron density of $\sim 10^{19} \text{ cm}^{-3}$ is formed at the cathode firstly and then at the anode [2]. The influence of conditions on the electrode surface on the dynamics of anode plasma formations was established. In the course of the experiments a complex of filamentary microstructure of plasma formations was also discovered. This structure represents a set of current channels of micron diameters is formed as the result of closing of spark channels between electrodes.

The present work was supported by the Russian Foundation for Basic Research (grants No. 17-08-01690, 18-32-00566, 18-02-00631).

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Investigation of microstructure of current channels in nanosecond air discharge by laser probing methods

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To study the microstructure of current channels developing during breakdown of air gaps with an inhomogeneous electric field distribution, laser probing techniques based on multi-channel multi-frame registration systems [1] with high spatial and time resolution were used. The data were obtained using the 6-channel 18-frame optical registration system with the spatial resolution of $\approx 2 \mu\text{m}$. The exposure time of each frame corresponds to the duration of the probe pulse of the laser—70 ps at a wavelength of 532 nm.

It was established that at the moment (with an accuracy of ≈ 0.5 –1 ns) of gap breakdown plasma with electron density of $\sim 10^{19} \text{ cm}^{-3}$ arises near the cathode surface. At the stage of closure of developed cathode and anode clots, a complex filamentary microstructure of the current channels with a high degree of ionization and gradients of the electron density arises. The set of filamentary channels ultimately forms a single spark channel connecting the electrodes. The work is supported by the Russian Science Foundation (grant No. 14-22-00273).

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Development and use of super-wide band antennas for registration of radio emissions of high-voltage laboratory atmospheric discharge

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To register radio emissions at the ERG facility, we developed a set of ultra wideband antennas. This allows you to register pulses with frequencies from 1.6 to 9.3 GHz with a standing wave ratio not exceeding 2. Input resistance is reconciled to a wave impedance of 50 Ohms by means of a quarter-wave line.

A characteristic feature of the discharge radio emission is its simultaneous generation with bremsstrahlung. We assume that the processes that generate these phenomena have similar, similar mechanisms. The measured radiation can be associated with the acceleration of electrons in streamers. We also noted that radio emission is formed in the form of successive pulses, the number of which coincides with the number of pulses of soft x-ray radiation. Both microwave and x-ray radiation are registered in the prebreakdown stage of the discharge development, reaching a maximum of power during the pre-pulse current.

The work was partially supported by the Russian Foundation for Basic Research (grant 17-08-01690).

Near-electrode plasma formation in the initial stage of high-voltage discharge in air

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To study the initial stage of discharge formation in air with high temporal and spatial resolutions, a laser shadow shooting was used (up to three independent laser channels with 5 ns, 20 mJ at a wavelength of 532 nm). The applied optical microprojection scheme allows to obtain an image with a resolution of $\sim 10 \mu\text{m}$ when the main lens is more than 1 m distance apart, which makes it possible to shoot under the conditions of applied megavoltage level voltage. The scalability of the phenomena occurring near the point at different geometric scales of the atmospheric discharge gap is studied. The dynamics of plasma formation near the tip is compared with applied voltages of 40 kV and 1 MV, at comparable average field strengths. The effect of the applied voltage front on the structure of the germinating channels is estimated. Gradients of electron density are visualized, mean and local current densities are estimated in the phase of formation and growth of discharge channels.

The features of plasma formation at the time of the onset of the growth of discharge channels can determine the properties of the radiation generated at this time [1,2]: the variation of the output of hard radiation on a large scale from shot to shot, complex spectral and angular distributions of emissions, etc.

The work was partially supported by the Russian Foundation for Basic Research (grant 17-08-01690).

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On pulsating neutron yield under inertial electrostatic confinement in vacuum discharge

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Neutrons from DD fusion in the interelectrode space of a small-scale low energy nanosecond vacuum discharge with a deuterium-loaded Pd anode have been demonstrated earlier (see [1] and refs). The goal of this work is to present and discuss in detail available experimental results on deuteron oscillations followed by pulsating DD neutron yield under inertial electrostatic confinement fusion (IEC) [2] based on nanosecond vacuum discharge. PIC simulations of some experimental regimes of pulsating neutron yield are presented. Comparison with available rather similar scheme of periodically oscillating plasmas spheres (POPS) [3] for IEC fusion is given and discussed also.

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Method for elimination of concomitant x-ray radiation from neutron generators based on plasma focus chambers

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Neutron generators on plasma focus chambers are sources of short, intense neutron pulses. The chamber of the plasma focus is a gas-filled chamber with a special design of electrodes connected by an insulator, the volume of the chamber is filled with deuterium or a mixture of deuterium and tritium. These facilities are used for research in various fields of science and technology: in studying fast processes, studying the interaction of neutron and x-ray radiation with matter, in pulse activation analysis, in dynamic radiography, for calibrating particle detectors, and so on. The generation of neutron radiation from the chambers of the plasma focus is accompanied by a flux of quanta of hard x-ray radiation of relatively large magnitude, which causes difficulties in recording the neutron pulse. In this paper we consider a method for eliminating the concomitant x-ray radiation, based on the modified electrode design of the plasma focus chambers.

Quantum dynamics of charged particles in Wigner formulation of quantum mechanics

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The dynamical electrical conductivity is of fundamental importance for the plasma behavior in a high-frequency electromagnetic field, in particular for the interaction of charged particles with intense radiation and for inertial thermonuclear fusion. There are many theoretical models of dynamic conductivity which can be derived from a kinetic theory. Molecular dynamics simulations of fully ionized classical plasma are widely used for the calculation of electrical conductivity with the help of the Kubo formula, but our main interest is to improve these results by taking into account bound states and quantum exchange-correlation effects. This can be done by means of Wigner approach to quantum mechanics. Combination of path integral Monte-Carlo method and Wigner dynamics, on the other hand, is free from these drawbacks and therefore can be used for the construction of a generalized molecular dynamics method for the calculation of electrical conductivity.

Numerical calculation of momentum distributions in non-ideal plasma

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In classical statistics at thermodynamic equilibrium all particles are maxwellian, but quantum effects may change this situation. The first mechanism is exchange interaction between identical particles, which turns maxwellian distribution into Fermi or Bose distribution. The second mechanism is Heisenberg principle: interaction of some particle with others reduces the available volume, which leads to uncertainty in momentum resulting in increased probability to have higher momentum. This effect was firstly predicted by Galitskiy for two component Coulomb system, it has been resulted in additive “tail” to maxwellian distribution function. Recently time Starostin et. all have explored the issue in more detailed way.

Unfortunately these results have been obtained using perturbation theory and are unsuitable for strongly coupled Coulomb systems. However regime of strong coupling is of the greatest interest, because it covers the most important applications: dense plasmas in astrophysics, electron-hole plasmas in semiconductors, etc. Therefore *ab initio* non-perturbative methods for calculation of equilibrium distribution functions are needed.

In our work we propose two numerical methods for calculation of equilibrium momentum distribution functions for strongly coupled two-component plasma. They are based on Wigner function in the phase space. We study momentum distribution functions and thermodynamics of hydrogen plasma and electron-hole plasma at coupling strength Γ from 0.8 to 2.0 with degeneracy of electrons $n_e \lambda_e^3$ from 0.3 to 5.

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Atomic and Coulomb models of systems with the Bose–Einstein condensate: Comparison, new results and peculiarities

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The new results on consideration of systems with the single-particle Bose–Einstein condensate (BEC) (superfluid helium (He II) and rarified Bose gases) are presented for two models: usual system of neutral atoms (atomic system) and Coulomb system consisting of electrons and nuclei which interact via Coulomb potential. For atomic system with the single-particle BEC the two different branches of elementary excitations were predicted in [1] and considered and justified in detail (see [2] and references therein): the collective phonon–roton excitations and the single-particle excitations with an energy gap. The first one is typical for liquids and conditioned by strong interatomic interaction. The last one is related to the BEC and conditioned by the basic Coulomb interaction potential between charged particles [3]. This interaction has no zero component, according to the condition for its Fourier component: $V_{a,b}(q=0) = 0$, where $a, b = (e, n)$ —indexes for electrons and nuclei. For atomic system the Fourier component of the short range effective potential U_{eff} for interacting neutral atoms should reflect this peculiarity of Coulomb interaction and also has discontinuity for $q = 0$. The low-frequency second-order singularity is found in the dielectric permittivity of a homogeneous and isotropic Coulomb system consisting of electrons and boson nuclei.

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The thermophysical properties of tantalum plasma

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The thermophysical properties (equations of state and electronic transport coefficients) of metals plays important role in different fundamental and applied tasks. Thus, there are many calculations and measurements at relatively low temperatures in solid and liquid phases. However, for the most of metals corresponding information at the high-temperature region (at $T \geq 5$ kK) is very limited (see, for instance, [1]). Moreover, the temperature can not be measured directly in the available experiments yet. Nevertheless, the available measurement data [2,3] allows one to check the existing calculation models.

Earlier we have developed a model to study the considered properties of metallic plasma. It gives the ionic composition, thermodynamical values and electronic transport coefficients. The model was applied to different substances, including noble gases, several metals and semiconductors (see references in [4–7]). It is based on the “chemical” approach (to find the plasma composition and thermodynamical values) and the relaxation time approximation (to find the coefficients). In present study it is applied to tantalum. The properties under study was calculated at $T \geq 10$ kK and densities $\rho \leq 4$ g/cc. The obtained results are in good agreement with available results of measurements and calculations of other authors.

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Simulation of dynamical properties of nonideal plasma by density functional theory and wave packet molecular dynamics methods

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In this work, we report on evaluation of different simulations methods for studying electron–ion non-ideal plasmas and warm dense matter. The internal energy and pressure are calculated using the classical molecular dynamics (MD), the wave packet molecular dynamics (WPMD) and the wave packet Monte-Carlo (WPMC). Constraining boundary conditions with a harmonic wall potential are used for wave packets to prevent wavepacket spreading. A combination of density functional theory (DFT) and WPMD methods is proposed to simulate the thermodynamics and the electronic dynamical properties of the nonideal plasma. In this approach we use the non-antisymmetrized single Gaussian wave packets to represent electrons and point-like particles for ions. The kinetic and electrostatic energy contributions for electrons are calculated within the WPMD model, whereas the exchange-correlation energy and its derivatives with respect to the dynamic variables is evaluated on a space mesh. The second result is concerned with determination of the area of applicability of the classical MD and WPMD-DFT. For this, the equation of state for hydrogen plasma was calculated for a range of densities from $n_e = 10^{21}$ to 10^{24} cm⁻³ and a range of temperatures from 10^3 to 10^5 K. The equation of state obtained by different approaches was compared with the ab initio methods such as path integral Monte-Carlo (PIMC). We show that at certain plasma parameters the MD method fails due to appearance of unphysical ordered structures of particles.

Comparison of warm dense hydrogen models: Wave packets and density functional theory

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Recent experimental results [1, 2] give the different conditions for fluid–fluid transition in warm dense hydrogen. Computer simulations can give important hints for solving this problem but the non-ideality effects and the effects of electron excitation should be properly considered. In this study, we consider two theories: the density functional theory (DFT) [3] and the electron force field (EFF) approach [4–6]. DFT works with electron density and is well tested for equilibrium systems. EFF is based on the Hartree representation of the electron wave function as a superposition of Gaussian wave-packets with the correction for Pauli exclusion. EFF allows us to observe non-equilibrium electron dynamics.

We have carried out equilibrium simulations of dense hydrogen at about 1.0 g/cm³ and temperatures about 2000–40000 K in both theoretical frameworks and compared the electron density distributions. We have also conducted MD simulations of the isochoric heating process in this temperature range and have analyzed ionization and dissociation processes. The results have been compared with the experimental data.

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Thermionic emission from surface of nanoplasma

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Nowadays interaction strong laser fields with nanosized objects is a very popular issue. As in the bulk case, the electromagnetic radiation can interact only with the electrons and causes their rapid heating and ionization of atoms. The result is the nanosized object with a relatively high electron temperature density and degree of ionization. It is called nanoplasma.

One of the distinguishing features of the nanoplasma is the violation of the plasma neutrality [1]. Due to the laser ionization and further thermionic emission from the plasma surface, the cluster gains an uncompensated positive charge.

This paper presents a theoretical model of emission current from nanoplasma. The model consists of a system of ordinary differential equations. The paper discusses the details of applicability of the model and its advantages and disadvantages. Comparison with a series of experiments [2, 3] is presented. The suggested system of equations allows generalizing the experimental results and giving a new explanation of them. Some of the presented results can be found in the article [4].

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Criteria of runaway electrons in a gas diode with a sharply nonuniform electric field

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The dynamics of runaway electrons in a gas diode in a strongly nonuniform electric field determined by the geometry of electrodes is considered. The obtained analytical solution of the equation of motion of electrons for an edge cathode shows that their runaway at the periphery in the region of weak field is possible only if the applied potential difference exceeds a certain threshold determined by the interelectrode distance and the parameters of the gas [1]. This condition supplements a classical runaway condition that the field strength at the emission edge of the cathode should be higher than a threshold value depending only on the parameters of the gas [2]. According to the estimates, this new condition imposes higher requirements than the classical condition on the field strength in the limit of the strongly sharp edge of the cathode.

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

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In the present paper energy distribution functions of fast particles, including primary and secondary electrons are calculated by PIC0 approach in the programming complex as a function of time in time interval from 10 ps to 10 ns, and in the range of neutron flux intensity time and space dependence. Self-consistent non-linear problems, such as electron ion recombination, value of electric field in the dated point and successive generation of secondary electrons are solved by Monte-Carlo technique and thoroughly described. Detailed calculations are shown and they were focused to detect the presence prove of so-called runaway electrons in the practical range of external electric field. In presented procedure clearly stated that there were no reasonable ways to transfer external electric field energy to primary electrons able to supply them relativistic energy and create runaway electrons, as it takes place within nuclear core in nuclear fission process, provoked by neutrons and antineutrinos. Time dependent spectra of primary electrons as well as their successive generations are calculated and compared with existing experimental data and Boltzmann kinetic equation solutions. Zero-point approximation developed in the present paper studies the point in the nuclear induced plasma under the condition, when the size of the point is much smaller than the size of experimental cell and where the statistical approach is reasonable and self-consistent electric field is the subject of energy distribution of electrons and positive ions.

Laser propagation in dusty quantum plasma with spin exchange interaction

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Two ubiquitous ingredients in the universe are plasmas and charged dust. The interplay between these two has opened up a new and fascinating research area, that is of dusty plasma, which are ubiquitous in different parts of our solar system, namely planetary rings, circumsolar dust rings, the interplanetary medium, cometary tails, as well as interstellar molecular clouds etc. Dusty plasmas also occur in microelectronic processing devices, low-temperature laboratory dusty plasmas devices, and in tokamaks. Dusty plasma is an ionized gas containing small particles of solid matter, each of which acquires a large electric charge by collecting electrons and ions from the plasma. Dusts are micron-sized particles that become electrically charged through interaction with the background plasma causing them to act as a third charged plasma species. Recently, a great deal of attention has been paid to quantum effects in dusty plasma.

The present paper is devoted to study of propagation of high intense electromagnetic wave in quantum dusty magnetoplasma having inertia-less degenerate electrons with spin-up and spin-down states. The effects of quantum Bohm potential, electron Fermi pressure and spin magnetic momentum has been analyzed taking into account the difference in spin-up and spin-down concentration of electrons caused by external magnetic field. The longitudinal dispersion relation for electromagnetic waves in dusty magnetoplasma has been setup and effect of spin polarization has been studied. The right circularly polarized, left circularly polarized wave, ordinary mode and extraordinary mode have been analyzed.

Effect of non-linear screening on thermodynamic properties of complex plasma

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Thermodynamic properties of equilibrium complex plasma and an applicability limit of the complex plasma well-known phase diagram [1] are under discussion. Present work is devoted to the analysis of the applicability range of a basic assumption in the phase diagram [1], i.e. linearized (Debye) screening of macroions by microions, which leads to the Yukawa form for effective interactions between macroions. Parameters of non-linear screening for macroions were calculated within a direct Poisson–Boltzmann approximation. Two basic effects were revealed as a result of such calculations: (i) decomposition of all microions onto two subclasses, free and bound ones, and (ii) significant reduction of effective charge Z^* of initial bare macroion Z under non-linear screening by small high-density envelope of bound ions. The effective charge Z^* grows as a linear function of Z first and then, the change of Z^* is negligibly thin. This renormalization of initial Z and macroion concentration n at the border of the cell into Z^* and n^* leads to corresponding renormalization of initial Γ and κ into Γ^* and κ^* ($\Gamma^* < \Gamma$ and $\kappa^* < \kappa$). The main physical assumption of the present work is that phase state of complex plasma under non-linear screening is still the same as in the initial phase diagram, but in $\kappa^*-\Gamma^*$ plane instead of $\kappa-\Gamma$ one. Corresponding calculated shifts of phase boundaries and excess internal energy in the initial phase diagram are discussed and illustrated. The work is supported by the Russian Science Foundation (grant No. 14-50-00124).

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Configurational entropy in dusty plasma model

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The thermodynamics (the entropy and thermostat models), statistical physics, concepts of equilibrium and partial equilibrium are crucial for dusty plasma description. The problem of estimation of dusty plasma entropy is under consideration. All approaches of this research are based on analytical and theoretical approach, and also on molecular dynamics simulation of dusty plasma system.

The divergence of trajectories of dusty plasma model system allows to calculate K-entropy (Krylov–Kolmogorov–Sinai entropy). The value of K is also equal to averaged maximum Lyapunov exponent and entropy growth rate since reciprocal is an important relaxation time. Furthermore, predictability time is studied. This time characterizes the time interval, during this interval future behavior of a dynamic system based on the initial conditions and deterministic dynamical equations can be predicted. The configuration entropy is compared with K-entropy.

The time of trajectories divergence in the molecular dynamics simulation might be different in different directions, so the partial equilibrium subsystem can be observed in the system. Estimations for the characteristic time of divergence in different directions of dust particles motion are obtained. The method for entropy is estimated for conditions of standard laboratory experiment on dusty plasma. The applicability of the thermodynamic functions for the description of plasma-dust system is discussed.

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Properties of dusty plasma structures under different discharge conditions

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In this work, dusty plasma structures are studied both experimentally (through the analysis of data provided by another group) and theoretically (using analytical, numerical methods and modeling). Average inter-particle distance dependence on the temperature of neutral gas in the discharge is measured from experimental data provided by I S Samoylov, V P Baev and A V Kirillin [1]. The form of the dependence discovers growth of inter-particle distance at low temperatures instead of expected decrease [2]. This effect is explained by the action of thermophoretic and ion drag forces in the radial direction of the discharge tube and their significant increase at low temperatures. The result is confirmed by solving the equation for the equilibrium of particles in the structures numerically and in molecular dynamics experiments.

The structural diagram of dusty plasma for the temperature range 9–295 K is obtained from the experiment. Areas of existence of anisotropic crystals, vertical chains and disordered phase are given in the coordinates “discharge current versus temperature of the neutral discharge gas” and “concentration of the neutral discharge gas versus temperature of the neutral discharge gas”. Areas of existence of multilayered structures and vertical chains are obtained from molecular dynamics simulations.

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Recombination waves in a complex plasma of non-self-sustained discharge

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A theoretical study was carried out on the phenomenon of the separation of stationary dust structures into regions with an increased and decreased concentration of dust particles, which was observed in complex plasma of a non-self-sustained discharge supported by a beam of protons. The discharge is used in the SSC RF IPPE to simulate nuclear-excited dusty plasma and to study its properties. The cause of stratification and the formation, as a result, of spatially periodic dust structures is recombination instability. The linear stage of instability and the physical mechanism of its occurrence are considered. The investigation of the stationary spatially periodic structures that are formed as a result of the development of the nonlinear stage of recombination instability in dusty plasma of a non-self-sustaining discharge is carried out. Two types of structures specific for a given discharge are identified—for small and large values of the recombination instability increment. Characteristic features of each type of structures are described and the mechanism of their formation is explained. It is also shown that the results of calculations are qualitatively and, with small variations in the discharge parameters, quantitatively comply with the experimental data.

Investigation of the vibrational properties of the dust particle in the stratified glow discharge

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Dusty plasma is a system, which is available for observation at the kinetic level, which makes it the basis for studying such phenomena as phase transitions, waves, instabilities and responses to different external influences [1]. The investigation of free and forced oscillations of dust particles is important for understanding the dynamics of dusty plasma. For example, the investigation of the oscillatory motion of the dust particles can be used to study the phenomena of energy transfer between degrees of freedom in a plasma–dust system [2].

In this paper, the method of the discharge current modulation [3], was used to investigate the vibrational properties of the dust particle in the stratified glow discharge. In the pressure range $p = 0.06\text{--}0.66$ Torr the amplitude–frequency characteristics of the single dust particle oscillations are obtained. The values of the vibrational characteristics of a dust trap such as eigenfrequency, and resonance frequency, Q-factor, damping coefficient are obtained. The calculation of the dust particle charge with the help of the experimentally obtained eigenfrequency is made. The obtained value of the dust particle charge is in good agreement with the literature data for similar discharge conditions [4].

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Ionization–recombination processes in non-linear dust-acoustic waves

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Long-wavelength high amplitude self-exciting dust acoustic waves in the gas discharge plasma are under consideration. A model included effects of the volume ionization and recombination on the dust grains is used for connection of the wavelength and the plasma parameters.

Lunar dust under investigation of future Russian space mission

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Under solar interaction and meteorite bombarding, the upper regolith level of the Moon becomes as aggressive environments with variable physical and optic properties. Low conductivities of regolith particles make it possible to be charged and save the charge during a long time. And low value of conductivity is able to have a significant photo-induced charge on a large area of the Moon surface. Closest Russian missions to the Moon with descent modules are Luna–Glob and Luna–Resource and they will have onboard the dusty plasma science instruments for investigation dynamics and properties of the Moon dust and electric fields. If future space missions are a happy scenario, we shall have data about dusty plasma and electric fields above lunar surface.

Dusty plasmas at Martian satellites

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We study dusty plasmas in the vicinity of Martian satellites Phobos and Deimos. We perform our research in connection with the future space projects “ExoMars 2020” and “Phobos-Grunt 2” which are now under development. We develop physical-mathematical models of dusty plasma systems in the vicinity of Martian satellites Phobos and Deimos and show that the dusty plasma systems include charged dust, photoelectrons, and electrons and ions of the solar wind. We determine the distributions of the photoelectrons and find the characteristics of the dust which rise over Phobos’ and Deimos’ surfaces. We compare the properties of the dusty plasmas at the Moon, Phobos, and Deimos. We emphasize that Phobos’ (Deimos’) gravitational pull is only a few thousandths of that at the Moon. This indicates the presence of significant features of dusty plasmas at Phobos and Deimos in comparison with that at the Moon. We formulate these specific features.

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Formation of clusters of diamagnetic macroparticles in colloid systems in magnetic traps

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The aim of the present work is to explore active particles in colloidal systems [1]. Particular interest in such systems can be caused by the research of phase transitions. The property of diamagnetic particles to be pushed out to the region of the minimum of the magnetic field is well known. Thus, for retention of dust structures and experimental research of strongly interacting Coulomb systems the levitation of diamagnetic particles in a nonuniform stationary magnetic field can be applied. At the same time, after the force of gravity, in ground experiments, when working with graphite particles, it is possible to form a cluster consisting of only a few particles [2]. In the present work the method of cluster formation in the laboratory conditions in a colloidal suspension situation, when the force of gravity, in accordance with the law of Archimedes, partially or completely can be compensated by the buoyancy force, was applied. To form a dust structure, the colloidal system is placed in an inhomogeneous magnetic field with a minimum of magnetic induction in its central part. Depending on the liquid particles of the colloid can be both neutral and charged. The phase transition in this system can be initiated by various mechanisms, for example, using laser radiation. In this case, the particulates can effectively scatter light. The possibility of video registration of the position of dust particles, at each moment of time creates a unique opportunity to explore the investigated system at the kinetic level.

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The calculation of the charge and dynamic characteristics of the dust particles for experiments in near-earth space

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Space experiment “Dust-UV” aims to generate and research plasma-dust formations, including those induced by uv radiation of the Sun (photoionized dusty plasma) in space. Preparing for the experiment quantitative analysis and numerical simulation of charging and dynamics of dusty particles at different distances from the Earth for different parameters of the surrounding plasma and dust components and various lighting conditions were conducted. Equilibrium charge of the dust particles from its height above the Earth’s surface for different particle parameters was calculated. Moreover, it was obtained numerical data on the dynamics of the dispersion of dust particles in near-earth space for different initial conditions of the problem. We have also analyzed the case of thin (optically transparent) plasma.

Application and diagnostics of low temperature dielectric barrier discharge plasma created by different sources

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Currently low temperature plasma has a wide range of applications. It used for sterilization [1], biological tissue regeneration acceleration [2], seed characteristics improvement [3], etc. Two plasma generator configurations are used in this study: float atmospheric discharge, and helium plasma jet.

Results of this study are giving a new insight in low temperature study area. Control parameters (voltage, electrode spacing, gas flow) variation makes possible to completely study received plasma. The most suitable regimes for biological object were examined. Temperature distribution and uv measurements allow to recognized safety of using it on living objects. Spectrum research got a data of plasma composition and measurements of plasma active components let to predict plasma properties and it influence on biological objects and tissues. Seed treatment is a first step of the plasma applying, which was investigated in this study.

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Phase transitions in two-dimensional systems with Yukawa interaction: Description by mean first-passage time dynamic entropy

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Dusty plasma of gas discharges is an excellent example of an open system far from equilibrium: for the existence of the discharge (i.e. for the levitation of particles) a constant energy supply is needed; during the experiment this energy dissipates on surrounding plasma particles. To study these systems properly, one should use methods independent of the degree of openness of the system and on the number of particles in it. One of the most natural methods to use is the concept of mean first-passage time dynamic entropy—a simple approximation of Kolmogorov–Sinai entropy [1,2]. In present work, the dynamical entropy of an extensive dissipative system with Yukawa interaction is studied numerically. Two parameters defining the state of a system—the coupling parameter and the scaling parameter—were varied in the wide range (from disordered to highly-ordered state of a system). For each state, the dynamical entropy of a system was calculated, the fractal dimension of grains trajectories and the size of their localization area were found. Two latter parameters appeared to have critical points in the vicinity of $\Gamma^* = 100$, that complies with the results obtained by the pair correlation function method. This work was supported by the Russian Science Foundation (grant No. 14-12-01440).

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Amplitude instability formation for Yukawa systems

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Conditions for amplitude instability formation in a system of charged grains placed in an external electric field are considered. Criterion for development of this kind of instability is proposed. The proposed analytical approach is tested by numerical simulations of problem for Yukawa systems consisting of two particles. Influence of formation of amplitude instability on the mass-transfer processes and on the dynamics of “leaps” in the two-particles systems is studied.

Exploring the wakes behind microparticles in the plasma sheath of an rf discharge

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Nowadays, there are no simple methods for exploring the wake-fields and measuring the wake-mediated interaction forces in complex plasmas. Most of existing methods require the experimental facility of special design that allows one to create an external perturbation of a particle system. They also often require preliminary measurements of electric fields and external forces acting on particles and prior knowledge of the plasma parameters and the form of interparticle interaction; and they can deal with one pair of dust particles only. In addition, the longitudinal distribution of the wake-fields in multiparticle dust chains in plasma has not been investigated at all. In this report, we propose an original method for exploring the wakes, which does not require any external influences on a system and does not rely on pre-measurements and any assumptions about the form of interaction.

For this, we extend the idea of correlational analysis of particles thermal motion in strongly coupled open dissipative systems [1] to study the nonreciprocal interparticle interaction in a many-particle system. Unlike the previous attempts to study the wake-mediated interactions in complex plasmas, our method does not require any external perturbations and is based on Brownian motion analysis only. The measurements were performed for the vertically aligned dust particles inside the glass box mounted on the lower electrode of RF gas discharge chamber. The experiment was conducted in argon plasma at 137 mTorr, monodisperse melamine formaldehyde particles having diameter of 8.93 μm were used.

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Influence of thermal motions on dynamics and diffusion of charged particles in the constant magnetic fields

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In the present work the study of dynamics and diffusion of charged particles in the constant electromagnetic fields are presented. The calculations were carried out for ions of different masses simulating uranium and its fission products in a typical range of parameters corresponding to the conditions of existent installations of spent nuclear fuel (SNF) separation.

It is shown that for the all cases the longitudinal coefficient of diffusion was equal to their coefficient of diffusion without magnetic field. At the same time the size of cross coefficient of diffusion corresponded to the Townsend ratio. It is necessary to emphasize that at the moment any information on numerical modeling of diffusion in a limited cloud of charged particles is absent.

For the first time an influence of thermal fluctuations of particles on their motion in an electromagnetic field is considered. Analytical estimations for the analysis of this effect are proposed. The proposed analytical relations were verified by numerical simulations.

In conclusion, the obtained results can be useful for an estimation of optimal parameters of power facilities that are needed for effective separation of ions in the SNF separation chamber. Besides that, the presented results can be also useful for qualitative analysis of weakly non-ideal dusty plasma behavior near the wall region of SNF installations.

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Brownian motion of a lone dust particle in plasma of rf discharge

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The motion of a lone charged microparticle levitating in the plasma of a capacitive high-frequency discharge at low pressure under laser action is studied experimentally [1]. For particles of various materials and properties of their surfaces the character of their motion via the parameters of the experiment is determined. It is shown that dust particles in gas discharge plasma can convert energy of the surrounding medium (laser radiation) into the kinetic energy of motion. The mechanism of motion for microparticles with a metallic surface is connected with photophoresis [2]. Absorption of laser radiation by the metal surface of the particle creates a radiometric force, which in turn makes the particle move. We observed experimentally the active Brownian motion (directed or irregular) caused by the action of radiometric force for various charged microparticles in the low-pressure plasma. At short time intervals, for particles with a metal coating, a direct motion with velocities up to 2500 $\mu\text{m/s}$ was observed; for large time intervals, the direction of particle motion is randomized, and the particle has a diffusive behavior of movements.

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Scenario of phase transition in a quasi-two-dimensional dusty plasma systems

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Recently, the study of phase transitions in the plasma-dust system causes a particular interest. Now, there are two main theoretical models describing motion in two-dimensional systems. According to one of them—the theory of Berezinsky–Kosterlitz–Thouless, the transition of a two-dimensional system from a crystalline state to a liquid state has a two-stage nature with the formation of an intermediate phase. Another theory of grain-boundary induced melting (GBI) does not consider the existence of an intermediate phase [1–3]. The present work is devoted to an experimental study of the phase transition in a dust structure with its partial heating. The experiments were held in the gas-discharge vacuum chamber with two electrodes in it. The plastic melamineformaldehyde particles, covered with copper (the layer of $9.95 \mu\text{m}$ thickness) were injected into the discharge chamber. A partial heating of the structure was affected by the action of a narrow-beam laser radiation of an argon laser on a dust monolayer. The obtained data was processed by the special script, and as a result, the following properties of particles were obtained: coordinates, velocities, trajectories and pair correlation functions.

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Interaction potential of two spherical macroparticles at constant surface potentials

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An interaction potential defines the rate constants of coagulation and agglomeration processes and determines the conditions of phase transitions in dusty plasmas and electrolytes. The purpose of this paper is a search for a simple method to calculate the interaction potential of spherical particles on the condition the surface potentials of the particles do not change in the change of the interparticle distance. This is satisfied by conducting macroparticles in any medium and also by any macroparticles situated in a uniform plasma or electrolyte where the surface potential of macroparticles is equal to the floating potential.

To find the interaction potential in uniform dielectric or weak screening plasma the capacitance and potential coefficients are used. These quantities are determined according to the asymptotical formulae [1, 2] for close approach of spheres and from the approximate formulae within the accuracy of R^{-17} for large interparticle distances R . In the intermediate region the capacitance and potential coefficients are found by matching the asymptotical formulae to the approximate ones. It has been established that this technique provides the precision high enough in the interaction potential calculation for all interparticle distances.

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Spherical macroparticles coagulation in a dusty plasma

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Nanoparticles are used in a lot of technical and medical applications thanks to their unique properties [1–4]. The coagulation or agglomeration of nanoparticles and their interaction with other objects are important in these applications. To describe electrostatic interaction of nanoparticles with the plasma screening effects taken into account, the model of two charged infinity parallel planes is widely used. In this paper the coagulation rate constant of spherical microparticles calculated in an equilibrium plasma or electrolyte including screening effects for the case of the weak and strong screening. The following two cases were considered: either the surface potentials or charges of microparticles are constant when the microparticles approach each other. Simple and rather accurate computation algorithms of coagulation rate constant are proposed. This work was supported by the Russian Science Foundation (grant No. 16-12-10424).

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Ionization rate and sputtering profile in dc magnetron discharge

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A relationship between the ionization rate distribution and the target sputtering profile in axially symmetric dc magnetron discharge in argon was studied. The distribution of the ionization rate was estimated from the argon ion glow. The use of a special diaphragm enhanced the effective dynamic range of the video camera, allowing simultaneous recording both a strong glow near the sputtering racetrack and a weak glow far from the cathode.

The work was supported by the Russian Science Foundation (project No. 16-12-10424).

Azimuthal inhomogeneities of axially symmetric rf discharge plasma in arc-shaped magnetic field

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The axially symmetrical rf magnetron discharge in argon with small admixture of air and in air was studied. The live plane electrode was equipped with ring-shaped dielectric insert. The electrode design of the magnetic system one allow the discharge ring locating in the region where the electric and magnetic field lines are not perpendicular to each other. In the case it was revealed that sectionalization of the glowing plasma ring takes place. Up to 10 long-living plasma bunches are observed. They locate equidistantly along the discharge ring and may either rotate around the discharge axe or rest. Both the discharge power and the working gas pressure are quite different from those proper to dc and high-power impulse magnetron sputtering discharges with spokes. The numerical modeling of the humid air discharge plasma was fulfilled and the ion composition of the plasma was determined. The plasma bunches formation mechanism and their rotation one are suggested basing on the numerical modeling results.

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Effect of pressure on the characteristics of dust particles in the the plasma of the proton beam

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In contrast to the previously performed experiments where dust particles have been obtained in tracks of accelerated protons we made a series of experiments using the accelerator of heavy ions EGP-15 (Electrostatic Charge-exchangable Generator with energy of accelerated ions up to 15 MeV). The accelerated ions of carbon 12 C have been used in the experiments. At first one-charged ions were accelerated (a charge is measured in the units of the electron charge). Then the ions went through the charge-exchange foil acquiring energy of 12 MeV at a charge of 3 and a value of the accelerating potential of 4 MeV. The ions arrived at the target unit going through the ion duct which was pumped up to the high vacuum condition. The experimental cell similar to the cell described in was installed at the target unit.

Virial equation of state for Columb system in Paul trap

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Virial equations of state of Coulomb systems were found. Coulomb system of similarly charged particles is unstable and in this work the system is retained in alternating electric field of a quadrupole type of the linear Paul trap. Simulation of Brownian dynamics of similarly charged particles in alternating electric field in air was carried out. Using the statistical theory of liquid state the analysis of stable oscillating system were provided and the equations of state for Coulomb system were found, such as energy U and pressure P of the system, virial equations $PV(\langle mv^2 \rangle / 2)^{-1}$. The Coulomb system is forced by external electric fields of the trap and oscillates that affect the equations of state of the system. The evolution of the equations of state of the Coulomb system as well as their dependence on the parameters of the system (particle charge and mass) has been studied. The virial equations of state of Coulomb systems were found. Coulomb system of similarly charged particles is unstable and in this work the system is retained in alternating electric field of a quadrupole type of the linear Paul trap. Simulation of Brownian dynamics of similarly charged particles in alternating electric field in air was carried out. Using the statistical theory of liquid state the analysis of stable oscillating system were provided and the equations of state for Coulomb system were found, such as energy U and pressure P of the system, virial equations $PV(\langle mv^2 \rangle / 2)^{-1}$. The Coulomb system is forced by external electric fields of the trap and oscillates that affect the equations of state of the system. The evolution of the equations of state of the Coulomb system as well as their dependence on the parameters of the system (particle charge and mass) has been studied. The work was done under support from the Russian Science Foundation (grant No. 14-50-00124).

Numerical investigation of the electric fields in the electrodynamic trap with a corona discharge

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Investigations of the structures of charged particles confined in traps of various types is the actual scientific task. Such structures can be obtained in low-pressure gas discharges [1] or using electrodynamic traps [1,2]. This paper is devoted to the study of a new type of trap, in which the electrodes of the trap also create a corona discharge. In contrast to classical electrodynamic traps, where the charge of particles remains constant, in the traps with the corona discharge particles are located in a medium containing positive and negative ions. The charge of the particle in this case depends on the strength of the electric field at the point of space where the particle is located. In this paper using numerical simulations we found the distribution of the electric field strength and the concentration of positive and negative ions in the trap region.

This work was supported by the program of fundamental research of the Presidium of the Russian Academy of Sciences No. 13 “Condensed matter and plasma at high energy densities”.

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Measurement of the charge of dust particles in the electrodynamic trap

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Investigation of the structures of charged particles is an actual scientific task. Such structures can be obtained using the electrodynamic traps [1]. In studies of this kind, it is important to obtain information about the parameters of the particles in the Coulomb structure. In [2] a method for measuring the charge and epy mass of single dust particles confined in a linear electrodynamic trap was proposed. However, this method is not applicable to Coulomb structures containing a large number of particles. In this paper, the charge of particles confined in the linear electrodynamic trap was determined from an analysis of the oscillations of the Coulomb structure under the action of an electric field. At both ends of the trap were placed additional electrodes. Rectangular electrical impulses were applied to these electrodes.

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Unstabilities in Coulomb structure

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The formation of wave processes in Coulomb system of charged particles was experimentally investigated in the linear Paul trap. Single autovawe that generated near the end of the trap and moved along the Coulomb system of trapped particles without damping was observed. The wave speed was determined and in assumption that the wave speed corresponds to the speed of sound and the approximation of a continuous medium of the structure the speed of sound was theoretically estimated. Theoretically estimated wave speed coincided with the wave speed obtained in the experiment. The theoretical study of wave generation was carried out.

Phase transitions in dust structures at cryogenic temperature

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In neon dc discharge at room temperature $T = 295$ K, the dust structures are formed from individual dust particles [1, 2]. The dust structures at $T = 77$ K can be multicomponent [1, 2], i.e. represent a mixture of dust particles and clusters formed by dust particles. In this work, the first- and second-order phase transitions in dust structures at $P = 20$ Pa and $T = 77$ K have been found. The experimental setup is described in [1, 3]. With increasing current, the complex clusters melted, producing a mixture of components consisting of simple clusters, complex clusters and individual dust particles. At $I = 0.631$ mA, the dust structure is in the crystalline state. The dust crystal is formed by cluster chains, which consist of multi-dimensional clusters. An increase in current to 0.633 mA is accompanied by a decrease and disappearance of the symmetry of the dust structure. Thus, the evidence of a second-order phase transition was observed. At higher current, a multicomponent mixture consisting of cluster chains and simple clusters was observed inside the dust structure, which indicated the mesomorphic state of dust system. At $I = 0.691$ mA, there was an abrupt jump in the dust structure volume, i.e. the density of the dust cloud decreased sharply, which indicated first-order phase transition. Here, the melting of complex dust clusters and partial melting of simple dust clusters were observed.

The present study was supported by the Russian Foundation for Basic Research (grant No. 16-02-00991).

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Spherical dust structures in cryogenic dc discharge in neon

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The spherical dust clouds were observed in gas discharges of various types, and their formation was associated with various conditions and discharge parameters. In our experiment, the formation of dusty structures of a spherical form in dc discharge in neon at a temperature of 77 K and a pressure of 0.14, 0.15, 0.42, 0.54, 0.9 and 1.2 Torr have been studied. At different values of pressure, the size of dust spheres varied and corresponded to different values of the discharge current. At all pressures, the spherical dust structures were in a liquid state. The spherical dust structures can be mono- or multi-component, i.e. represent a mixtures of dust particles and clusters formed by dust particles [1,2]. Components can be in motion. Apparently, the composition of dust spheres and various dynamics of the components, determined the nonmonotonic dependence of dust spheres size versus the discharge parameters. Dust spheres of different sizes are characterized by different surface tension. For the dust structure in liquid state, the surface tension can be represented through the binding energy of dust particles [3]. The binding energy of mixtures is different as the result of different total charge of components. Dust structures with dynamically unstable components have a lower binding energy than structures with the stronger interaction.

The present study was supported by the Russian Foundation for Basic Research (grant No. 16-02-00991).

- [1] Polyakov D N, Shumova V V and Vasilyak L M 2016 *J. Phys.: Conf. Ser.* **774** 012181
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Simulation of transition toward hollow dust structures in neon dc discharge

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The diffusion-drift model of the plasma of a positive column of dc glow discharge in neon with microparticles have been implemented for the simulation of the boundary of the transition from homogeneous to hollow dust structures, depending on the gas pressure and the discharge current. Simulated were the experimental data obtained in a discharge with a diameter of 16.5 mm with dust particles of 2.55 and 4.14 μm in diameter, at $P = 20\text{--}190$ Pa. As a criterion for formation of hollow dust structure, there was accepted the formation of the minimum on the profile of potential energy of dust particle in the net force field, that was a sum of forces of radial electric field, ion drag and thermophoresis. Simulations confirmed the experimentally observed decrease in the discharge current of a transition to hollow structures with increase in gas pressure. It has been shown that the magnitude of thermophoretic force is comparable to that of radial electric field and may be higher than ion drag force. The value of the thermophoretic force in the investigated range of parameters of the plasma-dust system was determined from the comparison of the simulated position of the hollow dust structure border with the experimental one. The results are relevant for the development of ideas about the fundamental forces acting on microparticles in plasma, and the improvement of plasma technologies. The financial support of the Program of basic research of the Presidium of Russian Academy of Sciences No. I.11P(1) "Thermal physics of high energy densities" is gratefully acknowledged.

Multiresonant anisotropic dielectric magnetic dipoles of elliptical form

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Experimental investigations of resonant phenomena in the electromagnetic fields generated by displacement current of elliptical close circuits were carried out at the excitation of lower resonant frequencies irradiated by the linearly polarized microwaves. Dielectric ellipse used in experiments is characterized by the dielectric permeability value of 110. It is external large half-axes $a = 2.8$ cm, small half-axes $b = 0.8$ cm, rectangle-shaped cross-section of ellipse with sides 0.5 and 0.8 cm. The spectral measurements had revealed the smallest resonance at the frequency value of 1.42 GHz. The smallest resonant frequency of elliptical dipole, induced by magnetic component of incident wave, is independent upon the dipole orientation with respect to the polarization of the incident wave. Besides the displacement currents, induced by magnetic component, the electric component of the incident wave generates a time-varying polarization in the parts of circuit, parallel to vector \mathbf{E} . Polarization currents induced by the electric component of vector \mathbf{E} are acting as the displacement currents exciting the magnetic responses of the circuit with different resonant frequencies, dependent upon the angle between the large axis of the ellipse and the direction of the wave propagation. Obtained experimental results clearly demonstrate the angular anisotropy of elongated elliptical dielectric magnetic dipoles, manifested in the dependence of their resonant frequencies upon the orientation of dipoles with respect to the direction of propagation of incident microwave. The work was supported by the fundamental research program of Presidium RAS No. 13 “Condensed matter and plasma at high energy densities”.

The removal of ammonia contaminants from the air flow by uv radiation

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The removal efficiency of ammonia contaminants from the air flow by uv radiation was investigated. The investigations were carried out on an installation with an ultraviolet reactor at an air flow rate in the range from 30 to 450 m³/h. A 120 W ultraviolet lamp generating uv radiation with two resonant wavelengths of 185 and 254 nm was used to remove ammonia. The ammonia concentration at the installation inlet was 100–200 ppm. The ammonia concentration at the outlet of the installation was determined by two methods—using an electronic ammonia sensor GasBadge Pro and using the Nessler chemical method. As a result of the work, it was found that the most effective removal of ammonia from the air is provided at normal humidity and is almost 2 orders of magnitude with ammonia concentrations at the installation inlet of about 10 ppm at the air flow of 55 m³/h. In humid air, the ammonia removal efficiency is about one order at ammonia concentrations at the installation inlet of 140–160 ppm at the air flow of cubic meter per hour. It is shown that the accuracy of measuring of the ammonia concentration in dry and moist air of the two methods corresponds to an error of not more than 20% (percents). This fact is satisfactory and corresponds to the error in measuring the Nessler method for the concentration of the reagent used.

Inactivation of microorganisms on plain dielectric surface by barrier discharge

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To study the disinfecting action of the plasma of barrier discharge on microorganisms used barrier discharge in a 0.25 mm gap between the flat surface of the metal electrode and the surface of a glass slide under normal air pressure. The test sample of the culture was applied in the center of a glass slide in the form of round spots with a diameter of 15 mm. To ignite and maintain a barrier discharge was used a source of high voltage sine wave with a frequency of 17.7 kHz with the ballast resistance for the desired current value. For the study used strains of microorganisms of the following types: spore-forming bacteria (*Bacillus pumilus*) and fungi (*Aspergillus niger*) isolated from the environment of the ISS. As a result of experiments it is established that the action of the barrier discharge is able to reduce the content on the dielectric smooth surface for a time from 0.5 to 60 s for two to three orders of magnitude the number of spore-forming bacteria and the three to four orders of magnitude the number of fungi. It is established that at the maximum level of initial contamination of samples high degree of inactivation achieved after 0.5 s. It is shown that upon further action of the discharge the degree of inactivation varies slightly.

Transitional regimes of pulsed electrical discharge in medium-conductivity water

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New regimes of pulsed electrical discharge development have been observed during experiments in water with conductivity $90 \mu\text{S}/\text{cm}$. At breakdown voltage U_{br} the discharge was found to follow “thermal” mechanism from anode similar to discharge in water with higher conductivity [1] with slight differences in time lags. Average plasma channel propagation speed at this conductivity was about several tens of m/s. Transition to three another “modes” of discharge, characterized by the higher average speed up to several km/s, was observed at the voltages above $\approx 2.8 U_{\text{br}}$.

The first “mode” initiates on anode as fast streamer discharge—leader-like structure with self-glowing shoots into the gap by 2 mm in first $10 \mu\text{s}$ at half voltage drop and transforms then into regular “thermal” mechanism finishing the gap breakdown in $\approx 1 \text{ ms}$.

The second “mode” initiates on anode as a thin, 0.3 mm length single streamer-like channel in first $10 \mu\text{s}$ which disappears rapidly at half voltage drop and the plasma channel develops only after long time ($\approx 2 \text{ ms}$) from cathode at the speed of several hundreds m/s. The third “mode” is a streamer-leader discharge with average speed of several km/s, known for low-conductivity liquids.

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Pre-breakout characteristics of weakly ionized media

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A system of equations for the pre-breakdown charge-formation in weakly ionized media was derived. From this system of equations, we obtained the conditions for quasineutrality and unipolarity for which the system decomposes into two simple subsystems. To analyze such pre-breakdown characteristics of weakly ionized gaseous media such as air it is reasonable to use unipolar system. Experiments with the corresponding measurements were carried out. Empirical current-voltage characteristics close to quasi-exponential curves were obtained. The dependence of the size of the zone of micro-breakdowns on the voltage was close to linear. The scheme of the experiments is presented. Analysis of the received results was carried out. It is shown that the results for liquids differ from the results for gases.

Influence of the growth rate of the voltage signal on the barrier discharge modes

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In the present work, modeling of atmospheric pressure barrier discharge in argon for a saw-tooth voltage signal applied to the electrodes was conducted. The model included balance equations for the densities of charged (electrons, ions) and the excited particles, the electron energy density, and the Poisson equation for the electric potential. The fluxes of charged (electrons, ions) and electron energy U_x were given in the drift–diffusion form. When using a linearly increasing voltage, the rate of voltage growth dU/dt is the one of the parameters regulating the discharge mode. As a result of numerical experiments, 3 various discharge modes were detected depending on the dU/dt , two of which are somewhat different kinds of Townsend discharge, and one form is a glow discharge. This work was supported by grants from the President of the Russian Federation (project No. MK-539.2017.1) and the Russian Foundation for Basic Research (project No. 16-38-60187).

Numerical simulation of the particle melting degree in argon plasma spraying

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In this work, the first model for the determination the temperature gradients within particles in a free jet was developed and simulated using a small and a large particle along their flight trajectory. To achieve this, three simulation models were coupled with each other. The first coupling took place between the simulation of the plasma generator and the free jet by exporting the flow profiles at the plasma generator nozzle as an inlet boundary condition for the free jet simulation. For the second coupling, gas temperatures and velocities at the immediate vicinity of the particle as well as particle velocity were used as boundary conditions for the transient heat transfer simulation within the particle along its flight trajectory. For the examined process parameters, the temperature gradients inside the small and the large particles diminish at around $L = 12$ cm from the nozzle and the temperature of the particles become uniform. The smaller particle is completely molten at the end of the flight trajectory, whereas the core of the larger one remains solid during the whole flight.

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Vitrification of fly ash from an incineration plant by air plasma

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The accumulation of a large amount of solid waste is a big environmental problem for mankind. There are a number of methods for their processing: combustion, gasification, fusion, etc. The most common method is burning, but during the processing ash is formed, which contains a large number of organochlorine compounds and heavy metals. Under the action of water, these substances can enter the soil and contaminate it. In this case, the most dangerous is fly ash, which has low resistance to leaching. One of the methods of processing fly ash can be plasma treatment. In most cases, studies are carried out by systems operating on inert gases. In the paper [1] melting of fly ash of the incineration plant is considered. The specific power of the facility was 3.2 W/g of ash. In another investigation [2], fly ash was exposed to dc argon plasma (20 I/min, 30 kW). In both cases, vitrified slag with high resistance to leaching was obtained. The experiment on air-plasma melting of fly ash obtained by burning the sewage sludge was carried out on the experimental IEE RAS facility. The produced slag was analyzed by the following methods elemental analysis (EDAX), x-ray diffraction analysis, IR spectral analysis, differential-thermal analysis.

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Features of CS₂ conversion in nonequilibrium gas-discharge plasma of multicomponent atmospheric-pressure mixtures

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Carbon disulfide CS₂ conversion in gaseous emissions is an important problem. We proposed to use a pulsed corona discharge to convert carbon disulfide in the air [1]. It was shown that the main products of CS₂ conversion are sulfur dioxide SO₂, carbonyl sulfide COS, sulfuric acid, and carbon dioxide.

It was detected that specific energy expenditures to remove CS₂ vary from 4 to 40 eV/molecule, depending on CS₂ concentration. Moreover, a mutual influence of CS₂, SO₂ and COS on the efficiency of the removal of all three toxic components exists. To solve the problem of optimization of pulsed corona discharge processing of air mixtures, a method of standard mixtures is proposed [1].

Air mixtures containing CS₂, SO₂ and COS at various concentrations were processed by pulsed corona discharge. Concentration dependencies of toxic impurities on the energy input into the mixture were obtained. It was discovered that to realize optimum removal of the toxic impurities from air it is necessary to vary parameters of pulsed corona discharge during the experiment.

This work was supported by the Russian Foundation for Basic Research, project No. 17-08-01212.

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Application of standard mixtures for the estimation of characteristics of non-equilibrium plasma of atmospheric pressure pulsed discharges

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Pulsed discharges of atmospheric pressure are widely used in plasma-chemical technologies. One of their important applications is the purification of air from the impurity of volatile organic compounds (VOCs). Nonequilibrium plasma, generated by the discharges, initiates the processes of oxidation and polymerization of VOCs in air flow without substantially heating the latter. This allows to develop on energy-efficient air purification technologies. In [1, 2] to estimate the efficiency of the use of a non-equilibrium gas-discharge plasma for air purification, it was proposed to use special mixtures of model VOC compounds with different functional groups. In this paper, we propose to use similar mixtures to determine the qualitative and quantitative composition of the active plasma components generated by the chosen experimental method. Different components react with plasma components at different rates, so the concentration dependencies of specially selected mixtures will reflect the composition of the plasma used. Thus, the use of mixtures of a special composition makes it possible to compare various technologies plasma-chemical technologies.

The work is supported by the Russian Foundation for Basic Research (project No. 17-08-01212).

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Overview of the heavy ion beam probe technical aspects on the T-10 tokamak

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Heavy ion beam probe (HIBP) is a unique tool for studying electric potential in the core and edge plasmas of the toroidal devices such as tokomaks and stellarators. Moreover, along with electric potential, HIBP gives information about the plasma density and the poloidal magnetic field. Measurements of all three HIBP quantities take place simultaneously and independently; it gives an important contribution to comprehensive analysis of the plasma turbulence.

After being formed in the emitter–extractor unit and accelerated in the injector, the probing beam enters plasma and moves along Larmour circle in a toroidal magnetic field of a tokamak.

As the primary beam passes through plasma, its particles are further ionized, doubly charged ions move along the trajectories with twice smaller Larmour radius and form a fan of secondary ions. Part of the secondary trajectories goes into energy analyzer, so only the particles from a given sample volume (SV) reach the detector.

The HIBP is a multicomponent diagnostics with many independent parameters. It consists of devices to form, accelerate, control and detect probing beam. The key issues we are facing with performing measurements are the high acceleration voltage, calculation of SV position and providing high precision and stability of accelerator and analyzer voltage. In this work, we describe technical development and the present condition of the Kurchatov Institute HIBP diagnostics placed on T-10 tokamak.

Study of the flow induced by surface dielectric-barrier discharge in electrode arrangement with an additional electrode simulating biological target

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When the biological target is not directly located in the discharge zone, there is a question of transport of the active components from the discharge zone to the processes sample. If a surface dielectric-barrier discharge (SDBD) is used as a source of ions and chemically active species, convective transport in the reactor is mainly due to the ionic induced by a discharge. We present the results of study of the structure of a discharge-generated flow in a plasma reactor, designed for biological samples processing. The study was performed using particle imaging velocimetry method. Reactor assembly included SDBD system and an additional electrode simulating a biological target (EST). SDBD was initiated in an electrode configuration of the “synthetic jet” type, consisting of series of parallel stripes. System was powered with sinusoidal voltage with frequency 5–30 kHz was applied to the strip electrodes; the response (buried) electrode was grounded. EST (grounded or biased by a constant voltage) was separated from the discharge by a gap of 10 mm. The dependence of the flow field structure on the separation between the strip electrodes, and on the magnitude of the bias voltage, is investigated.

Influence of front steepness of impulse voltage with nanosecond front duration on surface discharge characteristics in air

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Experimental investigation of a surface discharge in air driven by impulse high voltage has shown [1] that there is a marked difference in the discharge current curves for the different slope steepness of the applied high voltage the other conditions being the same. The present contribution deals with a surface discharge in air that appears at the edges of electrode placed on the surface of an Alumina plate. The other electrode is placed at the reverse side of the plate. The discharge is formed by two types of high voltage: a sine one with 14 kHz frequency and a periodic unipolar impulse voltage of the same frequency and the same amplitude. The voltage impulse duration in microsecond range and the impulse front steepness in nanosecond range are varied. The discharge current and voltage oscillograms and the discharge structure pictures made by digital photo camera are analyzed for a range of voltage impulse duration and front steepness. The experiments show that the discharge current in the oscillograms has a form of a number of discreet current pulses for voltage impulse front steepness less than 40 V/ns. An increase of the steepness up to 80 V/ns leads to an emergence of one single current impulse with high amplitude and duration about 30 ns. The discharge structure pictures show in all cases a channel form of the microdischarges but with low steepness branched channels are seen whereas with high steepness there are seen many thin close located channels that form practically uniform plasma layer.

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The formation and development of microdischarge channels in air near the surface of a dielectric barrier

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Results of some experiments aimed to clarify the location of surface microdischarge channels are presented. Some data about the location of the microdischarge channel has been presented in [1] where the distance L from the discharge channel to the barrier surface is evaluated as $200\ \mu\text{m}$. Experimental evaluation of the distance value L done in [2] on base of the channel light emission measurements gives at least $L = 1.5\ \text{mm}$ for dried air normal conditions. To clarify the problem some additional experiments were carried out with a single strip electrode placed on the surface of an Alumina plate barrier and the other electrode placed on the reverse side of the plate. A single impulse of high voltage with 30 ns front duration, $T_{\text{imp}} = 350\ \text{ns}$ and $U_m = 6\ \text{kV}$ was used to create the discharge. To check the possible location of the discharge channel a Plexiglas plate (a probe plate) was placed at different distances parallel the barrier surface (0.3–2 mm). After the discharge took place the surface of the Plexiglas plate turned to the discharge was processed with charged dust to develop possible traces of the discharge products. The results achieved with different voltage amplitude, different distance L of the probe plate to the discharge barrier surface show that the location of the surface discharge channel in the described conditions can be at least 0.8–1.8 mm away from the barrier.

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Convective thermal diffusion model of the hydrogen isotope desorption in the cathode spot of a vacuum arc with a ZrD_x cathode

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Although the use of neutron tubes with arc source of deuterium ions has been developed for nearly half a century, the mechanism of desorption of hydrogen isotopes from deuterated cathode in arc discharge is not studied yet. Today, it is considered that the main suppliers of deuterium ions in plasma of arc source are cathode spots (CS) [1]. This work has developed model of convective thermal diffusion of deuterium and desorption of deuterium into the CS plasma of the vacuum arc with a ZrD_x cathode. It was shown that limiting factor, which mainly determines deuterium desorption in hydrodynamic stage of functioning of cathode spot cell, is its transfer in the cathode from the volume to the surface. High gradient of hydrogen isotope concentration near the surface is maintained by pressing of almost desorbed surface layers of molten metal to crater peripheral area. Cathode volume, from which the gas is completely desorbed, is approximately equal to the volume of molten mass, pressed out upon formation of crater. Convective nature of deuterium desorption upon formation of microcrater results in the fact that the number of deuterium ions is by 4–6 times larger than the quantity of zirconium ions in CS plasma of vacuum arc with $\text{ZrD}_{0.67}$ cathode.

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Modeling of a micro tip explosion during a radiofrequency breakdown

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Numerical modeling of the electrical explosion of a micro-tip on the cathode surface with a high-frequency current was carried out. It is assumed that this phenomenon can be observed in the accelerating structures of TeV linear electron–positron colliders (CLIC) [1]. The CLIC accelerating structure, which is made of copper, operates at 11.994 GHz. The simulation was performed using the two-dimensional magnetohydrodynamic code [2], which used wide-range equation of state and the table of conductivity of the metal based on experimental data [3]. It was assumed that on the surface of a flat Cu cathode there is a microprotrusion shaped as a cylinder of radius $0.3 \mu\text{m}$ and length $1.5 \mu\text{m}$. The diode is connected in a circuit under maximal voltage 3.2 kV; the external resistance of 1 k Ω was chosen so that the circuit current in short-circuit mode was equal to 3.2 A. The work is supported in part by grants from the Russian Foundation for Basic Research (No. 16-08-00969, 17-08-00459 and 17-08-01282) and the President of the Russian Federation (No. SP-951.2016.1).

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On the mechanism of the initiation of an arc discharge on a nanostructured W-fuzz surface

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A key problem in the creation of the International Thermonuclear Experimental Reactor (ITER) is the choice of materials for the first wall and the divertor. The plasma-facing materials must withstand pulsed loads incommensurable in energy with the loads occurring in existing plasma installations. At the same time, they should be reasonably long-living to avoid frequent replacement of components. Intense plasma flows striking a material surface may initiate unipolar arcs, which are an extremely undesirable phenomenon. In an arc of this type, the current closes to the same electrode where the cathode spot has been formed; so these arcs were called unipolar. Experimental modeling of the physical processes in tokamaks revealed the formation of nanofiber layers on the metal surfaces subject to the action of plasma in tungsten-plate-helium-plasma contacts. It was observed that a surface structure of this type was formed at a high temperature of the plate exposed to an intense flow of low-energy (several tens of electron-volts) plasma ions. The nanofibers that covered the entire surface of the plate were named W-fuzz. Based on the available experimental data, the threshold values have been estimated for the main parameters characterizing the initiation of arc discharges on W-fuzz surfaces, namely the external energy load, the helium plasma flux, the potential of the plate, the discharge current, and the thickness of the nanostructured layer.

Improvement of inductively coupled plasma discharge by alternating-sign magnetic field line curvature

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Connection of the convex and concave parts of the field lines results in a reduction of the space charge that drives the unstable $\mathbf{E} \times \mathbf{B}$ motion, as there is an opposite direction of the particle drift in a non-uniform field at convex and concave field lines. The pressure peaking arises at the minimum of the second adiabatic invariant $J = \int v_{\parallel} dl$ that takes place at the middle of a tandem mirror-cusp transverse cross-section. The simple ideal magnetohydrodynamic (MHD) description gives a strong variation in the stable pressure profile due to the strong variation in the specific volume V : the critical profile being $p_{\text{MHD}} \propto V^{-5/3}$, where $V = \int dl/B$. However, we have found that there is a strong variation in the stable pressure profile at regions of almost equal specific volume, near $\min V$, with curvature of alternating sign—with appropriate combination of the convex and concave field line parts. For experimental research of this effect an inductively coupled discharge device has been used. Its magnetic configuration was improved by additional coil system to fulfill the alternating-sign curvature of magnetic field line. It has been found from the measurements of the transverse profiles of the ion saturation current that it increases substantially near the axis, where maximal mirror ratio takes place in the configuration of tandem mirror-cusp. Similar tendency of the ion saturation current increase was found in our previous study in electron-cyclotron resonance discharge [1]. Work was supported in part by the Russian Foundation for Basic Research, grant No. 16-08-01306.

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Splashing criteria for a molten metal in vacuum arc discharge: Cyclic processes in a cathode spot

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Liquid metal extrusion from craters, which are formed on the cathode during vacuum arc burning, is considered. Using the hydrodynamic similarity principle, this process is compared with the well-studied splashing process [1] that can develop within the impact of drops impinging one by one on a solid surface (the arc cycle duration is identified with the inverse frequency of the drop train). Based on this analogy, the conditions under which the regime of spreading of a liquid over the cathode surface will change into the splashing regime (accompanied by the formation of microjets and droplets) are analyzed. As it turns out, the conditions realized in vacuum arc cathode spot at near-threshold currents are close to the splashing threshold of liquid metal (see also [2]). This gives grounds to relate the existence of a threshold arc current [3] to the existence of a threshold for the process of liquid metal jet formation.

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Quasi-steady plasma accelerator as an injector for thermonuclear installations

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The study of the two-dimensional axisymmetric plasma flows in the channel of the quasi-steady plasma accelerator (QSPA) considered as an injector for the magnetic traps was carried out on the basis of the set of the magnetohydrodynamic equations taking into account the electrical conductivity, thermal conductivity, and radiation transport. The values of the discharge current in the accelerator are determined to ensure at the outlet the ion energy at the level 30 keV that is necessary for the subsequent fusion reaction of the D–T plasma in magnetic traps for plasma confinement. It has been established that a decrease in characteristic concentration of plasma supplied into the channel of the second stage of the QSPA makes it possible to substantially reduce the discharge currents which are needed to achieve thermonuclear parameters of the flow at the outlet from the plasma accelerator.

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Spectroscopic investigation of Hall and helicon grid thrusters and low-temperature xenon-lamp plasma

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In the paper, three type of xenon plasma (Hall-effect thruster (HT) [1], helicon grid thruster (HGT) and xenon lamp) were investigated by spectroscopic measurements in the 250–1100 nm range. So 42 levels and more than 90 transitions of Xe I and 64 levels and more than 150 transitions of Xe II and 3 levels of Xe III were observed. The experiment was conducted in the MIPT plasma propulsion laboratory. The experimental facility and methodology is discussed in detail in [2]. Emission of HT and HGT has several differences, but in both cases spectral lines responsible for heavy particle interaction and recombination are there. As expected the xenon lamp spectrum has other structure: spectral lines related to heavy particle interaction and high charged ions are poorly expressed. The state vectors [3] were obtained and compared. In general plasma of electric propulsion thrusters cannot be describe in the coronal model, but there are some transition that may be used for estimation of plasma plum parameters.

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Mathematical modelling of rarefied rf plasma flow with electrodynamics

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Radio frequency (rf) plasma at low pressure ($p = 0.15\text{--}150$ Pa) with gas flow is effectively used to modify the surfaces of materials of organic and inorganic nature [1, 2]. Plasma of this type has the following properties: electron concentration $10^{15}\text{--}10^{19}$ m⁻³, degree of ionization is $10^{-4}\text{--}10^{-7}$, the electron temperature is 1–4 eV, the temperature of the atoms and ions in the bunch $(3\text{--}4) \times 10^3$ K, in the plasma jet $(3.2\text{--}10) \times 10^2$ K. The rf plasma neutral component stream is in a transitional mode between the continuum mode and free-molecule flow, the electron component, metastables component and electromagnetic field can be approximated of continuous medium. Mathematical model of rf plasma flow at low pressures with influence of electromagnetic field is constructed. Calculations of rf plasma flow at low pressure are completed. The distributions of the velocity modulus, pressure and temperature of the carrier gas and the electron density, electron temperature, metastable density, electric field intensity are obtained. The reported study was funded by the Russian Foundation for Basic Research, grant No. 16-31-60081.

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Development of large-scale instabilities in the process of electrical explosion of profiled cylindrical conductors

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The paper presents the study of dynamics of large-scale instabilities that develop during the electrical explosion of profiled cylindrical conductors. The experiments were carried out on the high-current generator MIG (the current amplitude up to 2.5 MA, the current rise time of 100 ns). The magnetic fields induction at the conductor surface was in the range from 200 to 800 T. The instabilities were recorded with the help of a four-frame optical cameral with an exposure of 3 ns per frame.

Experimental modeling of lightning strike in soil

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Providing reliable transmission of electricity to the consumer is an important task of modern electric power industry. The impact of lightning strikes on objects of electric power facilities should be minimized; therefore each part and this system as a whole should be tested for resistance to lightning, including a protective grounding system. The length of power lines can reach thousands of kilometers. On the territory of the Russian Federation there are soils of high and low conductivity, and this must be taken into account when designing protective grounding systems. To carry out measurements of pulsed electrical ground parameters, a mobile test system was created, which allows working autonomously in the field for a long time. The system can create a current pulse discharge with an amplitude of up to 100 kA in the ground, and can measure electrical parameters of discharge.

The pulse value of soil resistance between metal rods placed in the soil to a depth of 1 m is obtained. This data indicate that spark channels can occur while current flowing through the soil. The presence of such channels is indicated by a decrease (2–3 times) in the resistance of the medium between the metal rods during the time of discharge of the lightning current. In the experiment, the arrangement of spark channels inside the ground was observed, as well as the escape of a spark to the surface. In the case of repeated breakdown in the ground, there was no noticeable change in the resistance between the grounding rods.

Arc initiation in plasma installations

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The paper is devoted to a research of electric arc ignition devices in plasma torch of an alternating and direct current. Initiation of the main arc becomes possible in several ways. One of them using ac plasma torch with rail electrodes [1]. Arc initiation in a zone of the minimum distance happens thanks to a plasma injector. High-voltage ac plasma is used as one of them. Its power is 5–10 kW, the plasma-forming gas flow 2–5 g/s. The plasma flow with electron concentration of $n_e = 10^{14}–10^{16} \text{ cm}^{-3}$ sufficient for main arc ignition is set in a zone of the minimum distance between the main electrodes of a plasma torch by injector operation. The second one using a construction series of the dc plasma torch. They were developed on the basis of a powerful three-phase plasma torch with rail electrodes [2], changing the installations power supply on a low tension to 1000 V. Their current voltage characteristics are received so as the resource researches. The cathode erosion is about $10^{-6} \text{ g/}^\circ\text{C}$, the anode is $10^{-7} \text{ g/}^\circ\text{C}$. The impulse erosive injector is developed for an arc ignition in a dc plasma torch. An impulse injector supply is carried out from the capacitive storage. At the same time the energy accumulated in the storage turns into discharge energy which is spent on the erosion of dielectric and electrode surface and also on heat-up and ionization of erosion particles.

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Plasma ways to obtain ultrafine oxides

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Plasma torch application in obtaining ultrafine materials has a wide number of advantages. First of all it is possible to provide high temperature of the chemical processes in a broad range of its values from 1000 up to 5500 °C. Secondary the process of the temperature regulation becomes simpler due to the modifiability of the plasma jet energy content. All this allows using an alternating current plasma torch for obtaining different ultrafine materials. The main part among demanded nanoparticles is made by oxides (61.3% in 1996, 73.4% in 2000 year). At the same time the amount of the most widely used oxides is SiO₂ (28.5%), Al₂O₃ (22.1%) and TiO₂(8.8%) [1]. Therefore the research of the process of obtaining metal oxides was made in IEE RAS [2]. Plasma chemical installation on the basis of a three-phase ac plasma torch [3] consists of the feed system of the processed material, a plasma torch, the plasma chemical reactor and the system of the end product collection. Plasma torch construction allows organizing the input of the processed material in several points along the plasma flow including directly in the arc chamber. Moreover the plasma torch casing is used as the first step of the plasma chemical reactor.

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Heat and dynamics effects in flow field formation by pulse periodic dielectric barrier discharge

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The surface dielectric barrier discharge (SDBD) actuators are considered as one of the prospective technique to improve the gas dynamic characteristics of the airfoil, to control the boundary layer characteristics and many others. The fundamental electrophysical and fluid dynamics nature of the processes and prospective of the corresponding applications based on such a discharge are studied intensively experimentally and analytically for recent decades (see, for example [1]). It seems that the most important feature of the phenomena involved is the multiscale character in both space and time behavior. In this paper, we present the results of the numerical simulation of the gas dynamics fields evolution in vicinity of the pulse periodic SDBD. The simulation is performed with in-house package PlasmAero. Several typical configurations of SDBD in a wide range of frequencies are considered. The evolution of discharge as well as the gasdynamic evolution of the flow field under periodic action of discharge is described. It was found that the near-wall jets are created both by heat release and by the electrostatic body force. The back influence of the gasdynamic evolution on the gas discharge feature is also found to be important. The new results obtained in this work can be important for many applications as well as for better understanding of the fundamental aspects of the flow interaction with the electrical gas discharge.

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The influence of magnetic field on the properties of high-speed plasma flows in magneto-plasma aerodynamics experiments

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Results of numerical and experimental study of a high-speed plasma flows created by magnetoplasma compressor (MPC) and pulsed discharge in capillary with ablating wall were presented in our previous works [1]. The possibility of using these sources for laboratory simulation of gas-dynamic effects and experimental study of processes of bodies interaction with hypersonic gas-plasma flows was shown. The range of speed and operating time of thus obtained plasma flows is 0.5–10 km/s and 0.01–50 ms respectively. The use of sufficiently low magnetic fields (0.5 T) in the wind tunnel experiment has a noticeable influence on the flow pattern in the vicinity of test bodies and on the regimes of heat and mass transfer and the radio waves propagation through a layer of thermal plasma created behind the shock wave. These questions are studied in more detail in this paper with variations in the plasma flow and the magnetic field parameters over a wider range.

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Theoretical research of interaction of an air stream with electric discharge in magnetic field

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Two-dimensional mathematical models of the interaction of airflow and a moving electric discharge between in an external magnetic field are presented in this work. The simplified two-dimensional models of longitudinal section and cross-section of the arc channel are formulated using equations of gas dynamics and heat transfer. Such approach together with thermal approximation of arc discharge allowed obtaining high spatial-temporal resolution. Volumetric force for simulation of magnetic field influence has been formulated as explicit function of temperature. For compliance to an experiment the integral of the channel current density was calculated at each time step of the calculation. The received total current of the discharge was compared to an experimental value. The analysis and verification of numerical calculation were made by means of comparison with simulation data obtained using program code PLASMAERO [1] and with results of experiments [2,3]. Two-dimensional longitudinal section of the arc channel was considered to investigate the influence of boundary conditions determined on electrodes. The problem was discussed using magnetohydrodynamic approximations and drift-diffusion approximation, and with taking into account influence of Hall current.

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Plasma jet control of the flow around the wing in subsonic flight

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Flow around the wings of an aircraft can be controlled by symmetric actuator dielectric barrier discharge (DBD). Lift force arises when the interaction between synthetic jet and airflow occurs. Lift force is significantly more, than thrust of the synthetic jet. For effective exploitation of DBD actuators as active flow control elements it is necessary to define places on the wing for better interaction of the synthetic jet with airflow. I.e. greater change of the lift force at constant linear thrust and specific thrust-to-power ratio of the synthetic jet.

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Spectral investigations of arc helium plasma: Density effects

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A study of the radiation properties of arc helium plasma of atmospheric pressure generated by a dc plasmatron has been performed. Electron number density and temperature and also populations of HeI atomic levels were determined from spectral measurements. It is shown that the arc helium plasma is nonequilibrium with a predominance of ionization over bulk recombination due to ambipolar diffusion from the discharge channel. The population of the ground state of HeI is almost two orders of magnitude higher than the Saha equilibrium one with respect to the ions and electrons. However the populations of the levels $n \geq 4$ are less than the equilibrium one and rapidly decrease with the approach to the ionization threshold. This is explained by the destruction of excited states due to the density effects, interaction with surrounding particles. The calculation using the model of the nearest ion microfield, which is successfully applied to many-electron atoms, gives a rather good agreement with the experimental data. At the same time, the uniform microfield model, giving good results for hydrogen plasma, in this case shows significant overestimation of the populations of highly excited states. The work was supported by the Russian Science Foundation, grant No. 14-50-00124.

Temperature field in the interaction region of high-enthalpy plasma stream and graphite surface

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Our group has designed and produced an experimental installation for studying interaction of high-enthalpy plasma jets with surfaces of heat-resistant materials. We used high-speed visualization, micro-pyrometric, spectroscopic methods to obtain data on spatial and temporal evolution of temperature fields on the surfaces of samples, mass loss dynamics and evolution of impacting plasma jet properties: electron temperature and concentration, heavy particle temperature. Plasma composition was determined by analyzing the emission spectra in the wavelength range from 250 to 450 nm where spectral lines of most molecular (C_2 , C_n , CN, ...) and atomic (C, Ca, ...) components appearing in the near-surface region during the sample destruction can be found.

When Nitrogen plasma is used, temporal and spatial concentrations of CN radical can be used as an indicator of the Carbon-containing sample destruction because this radical appears in the process of both surface carbon nitrification $N + C(\text{solid}) \rightarrow CN + 0.35 \text{ eV}$ [1] and similar gas-phase reaction in which plasma Nitrogen interacts with the atomic carbon molecules ablating from the heated surface of the graphite sample. A spectral band in the violet part of the visible wavelength range corresponding to the $B^2\Sigma - X^2\Sigma$ transition can be compared to a calculated one to find the parameters matching the experimental ones.

This work was partially supported by the Russian Foundation for Basic Research, grants No. 16-08-00323 and 16-08-798.

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Radial distribution of the electric field in a reflex discharge with multi-ringed electrodes

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Currently, there is little known about the establishment of a defined profile of the electric potential in the plasma. This is one of the key problems in the method of plasma separation [1]. While the end electrodes of the plasma separator is fed negative voltage, the vacuum chamber is grounded, which leads to the emergence of reflex discharge. This discharge generates a profile of the electric plasma potential. The work is devoted to the study of this profile.

Electrodes are placed at the ends of the cylindrical chamber (length 1.2 m diameter 0.85 m) create electric potential distribution. In this work, 7 coaxial electrodes are located at each end (the outer diameter of the assembly is 780 mm), each electrode has the form of a truncated cone. In this paper various configurations of voltage distribution on end electrodes are considered. The radial distribution of the plasma potential is obtained by the floating probe method and the radial distribution of the plasma density and electron temperature by the double-probe method. The region of the largest electric field and the boundary of the area of a “dense” plasma are determined.

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Line-ratio method for measuring electron temperatures of argon rf plasma in magnetic field

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Plasma separation method of spent nuclear fuel (SNF) [1] implies a spatial separation of low-temperature SNF plasma into two groups of ions which have different masses in presence of buffer plasma. The buffer plasma provides the compensation of spatial charge and creates electric potential required for the plasma separation. Also the buffer plasma must not lead to additional ionization of ions were separated, therefore we have to monitor the electron temperature. For this purpose emission line-ratio method was used [2]. In this work optical diagnostic of inductively coupled rf plasma (5 MHz) in magnetic field (650 G) was carried out. The chamber of plasma separator was evacuated to pressure 5 mTorr. Corona model for the description of emission processes in plasma was used. An average effective electron temperature was obtained (5 eV) by the argon 763.5–811.5 nm emission line-ratio method (level 2p₆ and 2p₉ respectively). For this purpose the excitation from the ground state and metastable levels was taken into account [3]. The obtained results are in agreement with data, measured from a double probe. The investigation is supported by the Russian Science Foundation, grant No. 14-29-00231.

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Optimization analysis of a plasma separator with a vacuum arc based plasma source configuration

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In the work, the comprehensive analysis of a plasma separator with a vacuum arc based plasma source is performed. The main purpose is to identify the interdependencies of the initial parameters set and separation rate to be able to optimize the configuration with the possible experimental limitations. The X - Y - Z modeling is performed with KARAT code [1] in a single-particle approximation. The basic configuration for the further analysis and optimization is taken from the work [2]. Injected particles are single-charged ions with energies from 0 to 20 eV with atomic masses $A = 150$ and 240 and spreading angle in the range of 0–30 degrees. Magnetic field is produced by 2 coils of wire, the characteristic field strength in an uniform area is 1–2 kG. Electric field is produced by several electrodes with electric potential up to 1000 V. As a result the correlations were identified and experimental configuration guidance was developed.

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Diffuse arc discharge with a hot cathode in a magnetic field as a plasma source of Pb and Ag mixture for problem of spent nuclear fuel reprocessing

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Conversion of a solid substance mixture into the low-energy (10 eV) plasma stream with stable parameters is a one of the important tasks for the developing nowadays method of plasma separation [1]. The study of plasma stream characteristics of Pb and Ag mixture was carried out. The evaporation of the substances was realized using induction crucible heating. The discharge was initiated by an electron beam. A variation of the thermocathode (LaB₆) temperature and the crucible heater power (vapor concentration) allowed to control the parameters of the discharge. It was shown, that maintaining a constant potential difference in the cathode-anode gap, in spite of the substantial difference in the saturated vapor pressure of model substances, is possible due to control of the thermionic current from the cathode. Measurements of the spectral composition of plasma radiation made it possible to determine the discharge burning regimes in which ions of multiplicity 2 were absent. The obtained results indicate the possibility of using this type of discharge for testing the method of plasma separation of spent nuclear fuel. The study was supported by a grant of the Russian Science Foundation (grant No. 14-29-00231P).

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