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The book consists of the abstracts of plenary, oral and poster contributions to the XXX International Conference on Interaction of Intense Energy Fluxes with Matter (March 1–6, 2015, Elbrus, Kabardino-Balkaria, Russia). The reports deal with the contemporary investigations in the field of physics of extreme states of matter. The following topics are covered: interaction of intense laser, x-ray and microwave radiation, powerful ion and electron beams with matter; techniques of intense energy fluxes generation; experimental methods of diagnostics of ultrafast processes; shock waves, detonation and combustion physics; equations of state and constitutive equations for matter at high pressures and temperatures; low-temperature plasma physics; physical issues of power engineering and technology projects.

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ON CORRELATION AND QUANTUM EFFECTS IN STRONGLY COUPLED PLASMAS

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The behavior of matter at extremely high densities is of high interest for understanding the structure and evolution of astrophysical objects and many modern energy technologies. Dynamic methods of generation of warm dense matter at extremely high pressures, based on the compression and heating of matter in intensive shock waves, adiabatic expansion of preliminary compressed matter and quasiisentropic compression are considered. To generate shock waves in the terapascal pressure range the cylindrical and spherical condensed high explosives, laser and corpuscular beams, high velocity impacts, and soft X-rays were used. The highly time-resolved diagnostics of the extreme states of plasma were carried out with differential laser indicators of velocity, fast acting electron-optical transducers, pyrometers, and high-speed spectrometers equipped with the electron-optical transmission lines. The experimental data obtained and the physical models of behavior of plasma at extremely high pressures, temperatures and deformation rates are discussed. These are the metallization and dielectrization of strongly compressed matter, high energy density thermodynamics and phase transitions, including plasma phase transitions. Shear viscosity of matter as an indicator of particles correlations in a wide region of parameters from Plank's scale to laboratory conditions is analyzed. Wide-range semi-empirical equations of state and models are constructed, which were used for multidimensional numerical simulation of pulsed high-energy processes and description of solar plasma. The role of the quantum and correlation effects in strongly coupled plasma analyzed on the base of the experimental data obtained.

INTENSE PARTICLE BEAMS AND HIGH ENERGY DENSITIES PHYSICS

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Day-one experiments with first heavy ion beam parameters at FAIR 2018–2022 suggested by HEDgeHOB collaboration in the field of high energy densities in the matter are discussed. The experiments on generation of high pressures and temperatures with the aid of heave ions and possibility of proton radiography on measuring of plasma parameters are considered.

INVESTIGATION OF THE SPALL STRENGTH OF GRAPHITE IN STRESSES PRODUCED BY NANO- AND PICOSECOND LASER ACTIONS

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On laser installations "Kamerton-T" (GPI, Moscow, Russia) and PHELIX (GSI, Darmstadt, Germany) spallation phenomena were studied experimentally in a graphite target with nanosecond and picosecond shock-wave action. In a range of strain rates from 10^6 to 10^7 1/s on the first data of dynamic mechanical strength of this material were obtained. Spalling was observed not only on the back side of the target, but also on its front surface. By using optical and scanning electron microscopy, ithe morphology of the front and back surfaces of the targets studied. A comparison of the dynamic strength of graphite with the dynamic strength of synthetic diamond was done.

THE BEHAVIOR OF METALS UNDER ULTRAFAST LOADS DRIVEN BY FEMTOSECOND LASER

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We report on the shock-wave phenomena in metal films of a micron or submicron thickness irradiated by femtosecond laser pulses. The single-shot ultrafast interferometric technique [1] was used to record the time and spatial resolved displacement of rear surface of the films. The free surface displacement histories were converted into the free surface velocity histories. As a result, new data on the HEL and spall strength values have been obtained for aluminum, iron and other metals in strongly metastable states close to ultimate shear and tensile stresses. Comparison of measured parameters of elastic shock waves with the data of plate impact experiments at larger sample thicknesses demonstrate different regimes of the decay: whereas for fcc metals the decay may be described by one power function over 10^{-3} mm to 10 mm range of the distances, in the case of bcc iron main decay occurs obviously at the distance of order of 0.05 mm [2], [3]. The data are discussed from the view point of main mechanisms of high-rate deformation and fracture.

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ABLATION OF TANTALUM IRRADIATED BY FEMTOSECOND LASER PULSES

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Our understanding of femtosecond laser interactions with metals based on the two temperature model [1]. Since the heat capacity of the electrons is much smaller than that of the lattice, an ultrashort laser pulse with a duration less than the heating time of the lattice can heat electrons in a metal

to a very high temperature while leaving the lattice relatively cool. Ultrafast heating the thin surface layer of metal target gives rise to powerful tensile stresses and ablation nanolayer of material [2]. In the current work ablation thresholds and morphology of the surface have been measured for tantalum by means of femtosecond interferometric microscopy [3]. Using an interferometric continuous monitoring technique, we have investigated the motion of the surface of a tantalum target in the case of femtosecond laser ablation at picosecond time delays relative to the instant of laser exposure. The experimentally determined value of the tensile stresses that lead to the separation of layer of material for different fluence. Measurements of the temporal target dispersion dynamics and the morphology of the ablation crater have demonstrated thermomechanical nature of the fracture of the condensed phase because of the cavitation-driven formation and growth of vapour phase nuclei upon melt expansion, followed by the formation of surface nanostructures upon melt solidification.

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DEVELOPMENT OF HIGH POWER TERAHERTZ FACILITY

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The novel facility for generation of high power subpicosecond terahertz radiation, not having analogues in the world, based on the unique terawatt femtosecond Cr:forsterite laser system has been developed in JIHT RAS. For the first time a record high THz pulse energy of 0.9 mJ with 3% efficiency in nonlinear organic crystals was obtained [1]. Extremely large field strength of 42 MV/cm with the potential to reach over 80 MV/cm was achieved. The developed facility opens new research areas of power terahertz-matter interaction, diagnostics of objects, including biological

and ultrafast processes dynamics.

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MODELING OF PUMP-PROBE EXPERIMENTS WITH Ti:SAPP PUMP AND X-RAY PROBE

Inogamov N.A.,[*1] ***Zhakhovsky V.V.,***[2] ***Khokhlov V.A.,***[1] ***Faenov A.Ya.,***[3] ***Shepelev V.V.,***[4] ***Ilnitsky D.K.,***[2] ***Hasegawa N.,***[5] ***Nishikino M.,***[5] ***Yamagiwa M.,***[5] ***Ishino M.,***[5] ***Pikuz T.A.,***[3] ***Takayoshi S.,***[6] ***Tomita T.,***[6] ***Kawachi T.***[5]

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Fifteen years ago observation and explanation of Newton rings [1] clearly manifests that ablation by an ultrashort pulse resulting in release of a spallation shell is qualitatively different from the gas-plasma flow ablation produced by a nanosecond pulse. Fast pumping of energy into material by an ultrashort pulse generates a state with pressure as high as in a detonation wave in high explosives. Strong shortening of pulse duration transfers a long pulse gas-plasma rarefaction wave to a rarefaction wave in condensed media where cohesive resistance to stretching plays a decisive role. All this is said to emphasize that the fast ablation is unique. Observations [1] have been made in a pump-probe scheme with an optical pump, wavelength $\lambda_{opt} \sim 1000$ nm. First rings appears when the spallation shell with velocity $\sim$0.5 nm/ps passes a distance larger than one half-wavelength $\sim$500 nm. Thus, observation of rings begins at $\sim$1000 ps after pump. In contrast, the new observation technique with soft X-ray probe $\lambda_X = 13.9$ nm allows to begin observations 1–1.5 orders of magnitude earlier. In the report the hydrodynamics and molecular dynamics simulations and their comparisons with X-probe experimental data are presented. We see how an internal ruptures appear and reflections from them begin to interfere. This sheds light onto dynamical effects accompanying cavitation and internal fragmentation of material. Support from Russian Science Foundation 14-19-01599 is acknowledged.

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THIN 10–100 nm FILM IN CONTACT WITH SUBSTRATE: DYNAMICS AFTER FEMTOSECOND IRRADIATION

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Ultrashort laser pulse may induce the interesting combinations of thermal and hydrodynamic phenomena including foaming and freezing of molten metals and semiconductors [1], formation of chaotic surface nanostructures and mesoporous layers [1], and superelastic shocks [2]. Appearance of negative pressures within the frontal surface layer heated by a laser has a key importance for understanding of frontal nucleation, foaming, and spallation often called ablation (mass removal) in laser community. Release and movement of spallation shell allows understanding the puzzle of Newton rings [3]. Disruption of a free-standing plane film quickly heated by a laser is the simplest model of laser spallation [4], in which the sharp spallation (ablation) threshold F_a determines dynamics of the free-standing film. Problem of significant importance is: how this picture will change if the film is deposited onto substrate? This problem is solved in the report. It is found that now there are two thresholds $F_s < F_a$ and three regimes of motion, comp. with the freestanding film. For $0 < F < F_s$ the film oscillates remaining on substrate. Oscillations decay in time due to emission of acoustic waves into substrate. For $F_s < F < F_a$ the film breaks away from substrate because negative pressure propagating with acoustic waves arrives to a film-substrate contact and overcomes the cohesion strength of the contact. In the third regime $F_a < F$ there is inner disruption of the film happened before a moment when negative pressure separates metal and dielectric substrate at the contact. Support from RFBR 13-08-01095 and RAS program “Substance at high energy densities” is acknowledged.

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IMPLEMENTATION OF NUCLEATION MODEL INTO HYDROCODE FOR SIMULATION OF LASER ABLATION

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We present a hydrodynamic model for simulation of laser–matter interaction. The model describes laser energy absorption, hydrodynamic motion of material, two-temperature effects, electron–phonon coupling and electron thermal conductivity. One of the basic mechanisms of femtosecond laser ablation is mechanical fragmentation. To properly take into account the nucleation in metastable liquid phase we implement into the hydrocode a nucleation model that takes account of formation of bubbles of critical size and their subsequent growth. During simulation thermodynamic parameters in metastable and stable phases are known from a multiphase equation of state. Results of modeling are in a good agreement with molecular dynamic simulation and experimental findings.

CONTINUAL ATOMISTIC SIMULATION OF METAL TARGETS IRRADIATED BY FEMTOSECOND DOUBLE-PULSES

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In this work, we study the mechanisms responsible for the dynamics of femtosecond double-pulse laser ablation of metals. In several experiments it was previously shown that the crater depth in double pulse irradiation monotonically drops when the delay between pulses increases. This decrease of the crater depth starts from the delay of several picoseconds and for delays longer than the time of electron–ion relaxation the crater depth can be even smaller than that produced by only a single pulse. To de-

scribe this complex dynamics we use an advanced specially developed hybrid method based on combination of atomistic and continual approaches. The atomistic system describes the evolution of a target irradiated by the laser pulses, takes into account melting, evaporation, nucleation and recoil effects while electronic subsystem is responsible for correct description of the laser energy absorption, thermal conductivity process and electron–phonon coupling. The results of simulation of the double-pulse ablation obtained for different delays from 1 to 100 ps correlate with the experimental findings.

MECHANISMS OF LASER PEELING OF THIN FILMS FROM SUBSTRATE AND FORMATION OF NANOBUMP

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The report is devoted to the studies of laser peeling of thin 10-100 nm films. To describe better the particularity of our subject, it is valuable to present shortly general picture of laser structuring. It is known, that the structuring of materials by short laser pulses with duration in the range of 10 fs - 1 ps has many important technological applications. But underlying physics is not well understood. On our view, the corresponding processes are some mixture and interplay of plasmon enhanced absorption from one side and a thermomechanical triplet from another side, where the triplet is: (i) spallation, (ii) capillary deceleration in tandem with (iii) diffusion limited freezing. Particular morphology of structures depends on absorbed fluence F_{abs} and number of pulses. Formation of the structures is usually attributed to plasmon activity, which leads to the LIPSS (laser induced periodic surface structures, ripples) [1]. On our opinion, plasmons only *dominate* in the interplay if absorbed fluences are small and multiple repetion is used. Indeed, the chaotic (not ripples) structures are produced by X-ray pulse where plasmon excitation is not possible [2]. Therefore the wavelength should be added into the list of parameters governing morphology of irradiated surface. It was shown [2] that for the small number of pulses, either large F_{abs} or short wavelength λ the chaotic structures different from ripples are formed. Another important governing parameters are connected with geometrical limitations. They are a radius of a focal spot R_L on a irradiated surface and film thickness which fixes spallation depth

if the film is mechanically weakly linked to a substrate. Indeed, surface structures have the finite lateral sizes of $\sim 0.1-1$ um. Therefore for tightly focused optical light pulses $R_L \sim \lambda \sim$ um, the structures have to change qualitatively, see [3] and Refs. therein. In the report the physics of the peeling is considered and the new (relative to [3]) results are presented.

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ATOMISTIC SIMULATION OF SURFACE MODIFICATION BY LASER PULSE: COMPARISON OF MODELS WITH VARIOUS SCALES

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In this work the femtosecond laser pulse modification of surface is studied for aluminium (Al) and gold (Au) by use of two-temperature atomistic simulation. The results are obtained for various atomistic models with different scales: from pseudo-one-dimensional to full-scale three-dimensional atomistic simulation. The surface modification after laser irradiation can be caused by ablation and melting. At low energy of laser pulse, the nanoscale ripples on surface may be induced by the melting without laser ablation. The nanoscale changes of the surface are due to the splash of molten metal under temperature gradient. The laser ablation occurs at a higher pulse energy when a crater is formed on the surface. There are essential differences between Al ablation and Au ablation. The swelling and voids formation as the first step at the shock-wave-induced ablation is obtained for both metals. However, the simulation of ablation in gold shows the existence of additional nonthermal type of ablation which is associated with electron pressure relaxation. This type of ablation takes place at surface layer, at a depth of several nanometers and does not induce swelling.

PERMITTIVITY OF HOT PLASMAS IN WIDE FREQUENCY RANGE

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Quantum statistical (QS) approach [1] for calculation of *intraband* part of permittivity ε of hot plasmas with different ions charges $Z \geq 1$ for wide range of densities and temperatures above 10 eV is considered for wide range of frequencies of laser radiation (from infrared to ultraviolet ones) and compared with approaches on the base of kinetic theory (KT) [2].

For laser frequencies ω_0 lower than plasma frequency ω_p and parameter of coupling $\Gamma_{ei} < 1$ the QS calculations of ε are in good agreement with KT results [2–5]. Particularly, use of Gould deWitte approach for calculation of the 1-moment correlation function and Screened Born approximation for calculation of renormalization factor [1] ensure results almost identical with ones obtained with wide-range kinetic model for $\omega_0 < \omega_p$ and electron temperatures T above 50 eV.

For $\omega > \omega_p$ use of Dowson-Oberman-like corrections [5, 6] to Coulomb logarithm in KT permits to describe real part of ε for $\hbar\omega_0 < T$, but for proper description of imaginary part of ε QS theory is needed. Also for larger values of laser frequencies $\hbar\omega_0 \gg T$ only QS theory can ensure proper description of bremstruhlang and gives right asymptotic expressions. Besides, QS theory describes consistently effects of electrons and ions correlations [7], static and dynamical screening and strong collisions. Influence of these processes and also of electron-electron collisions and modification of screening in plasmas with complex ions [8] is discussed.

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THE TRANSPARENCY OF POLYCAPILLARY SYSTEM 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 10nJ per impulse with beam focusing to spot size 1.3 μm gives electric field with tension $|E| = 1.2$ V/Å. This field is enough to produce ionization of inner surface atoms and surface plasmons generation. Also temperature dependence of adsorbtion spectra is investigated as was done in [1].

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ON THE POSSIBILITY OF HARD K_α YIELD ENHANCEMENT USING MICRO-STRUCTURED FOILS

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Developed model of K_α generation under vacuum heating of electrons near the surface of spherical clusters, covering a solid or a foil, by a femtosecond laser pulse with moderate intensity describes the measurements of hot electron temperature and the enhancement of the yield of K_α photons with energy 1–8 keV. When the laser field interacts with nanocylinders,

arranged on a foil, the K_α yield increases by more than an order of value compared to using the foil, covered with closely packed spherical clusters, in view of the optimal conditions.

Sources of high-energy K_α photons based on the use of high-intensity lasers are being developed to probe millimeter sized, high-Z and dense materials for the high-energy density experiments. Modeling of the yield of K_α photons with energy 68.8 keV from the front and rear sides of a gold foil of arbitrary thickness by perpendicularly incident, single-pass electron with an energy up to 10 MeV was carried out. Calculations show that the K_α yield can be increased at optimal foil thickness about 500 μm by increasing the number of hot electrons with the energy above 1 Mev. Available hot electron spectra obtained with 2D PIC simulations [1] indicate that this possibility can be realized by irradiation of wavelength-sized polystyrene spheres, deposited on the foil, by a femtosecond laser pulse with relativistic intensity.

The Russian Science Foundation has supported this work by agreement with JIHT RAS (grant No. 14-50-00124).

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QUASIMONOCHROMATIC BEAMS OF ACCELERATED ELECTRONS IN THE INTERACTION OF A WEAK-CONTRAST INTENSE FEMTOSECOND LASER PULSE WITH A METAL FOIL

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The formation of monoenergetic beams of accelerated electrons by focusing femtosecond laser radiation with an intensity of the order of $10^{17} W/cm^2$ onto the edge of aluminum foil was demonstrated in the experiments [1]. The electrons had energy distributions peaking in the 0.2 to 0.8 MeV range with a small energy spread about 20 percents.

The acceleration mechanism related to the generation of a plasma wave as a result of self-modulation instability of a laser pulse [2] in a dense plasma formed by a prepulse is considered. Three-dimensional PIC simulations of the laser pulse interaction with inhomogeneous plasma showed that effective excitation of a plasma wave as well as trapping and acceleration of an electron beam with an energy of the order of 1 MeV may occur

in the presence of sharp gradients in plasma density and in the temporal shape of the pulse.

Under experimental conditions the inhomogeneities in the temporal envelope of the laser pulse may be caused by ionization nonlinearity of the plasma formed by the prepulse, and the spatial density inhomogeneities may be due to the sharp boundaries of the foil and the complex configuration of the plasma spread.

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3D PIC MODELING OF ION ACCELERATION FROM A THIN PLASMA LAYER WITH OVERCRITICAL DENSITY UNDER THE ACTION OF SHORT INTENSE LASER PULSE. CONVERGENCE OF RESULTS DEPENDING ON THE COMPUTATIONAL PARAMETERS

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Development of the laser-plasma method for producing ion bunches with a high quality and sufficient total charge is relevant for different applications. To adequately estimate the energy of accelerated ions for given parameters of the laser-plasma interaction it is important to carry out three-dimensional calculations. 3D PIC modeling of real experimental setups is not yet fully mastered as it is highly computational resource consuming. When considering the overcritical target densities resource expensiveness is caused by the need to resolve small spatial scales associated with the skin layer $\sim c/\omega_p$, the Debye radius $\sim \upsilon_T/\omega_p$, target thickness of 5–200 nm and also the corresponding time scale. Here c is the speed of light, ω_p is the plasma frequency and υ_T is the thermal electron velocity. It is now possible to conduct simulations on modern supercomputers using highly scalable 3D PIC codes with required computational parameters close to the above described. However, the question arises under what computational parameters (cell size, the number of particles per cell) the convergence of calculation results to the mathematical solution of the problem with a given accuracy occurs. When answering this question, we can understand the extent to which we can rely on results of 3D PIC simu-

lations in describing and predicting real experiments. The results of the study of convergence of 3D PIC calculations depending on computational parameters for the model problem of ion acceleration from a thin plasma layer with overcritical density under the action of relativistically intense short tightly focused laser pulse is presented. It is shown that the convergence within 5% precision requires to resolve the skin layer and the Debye radius with at least a few grid nodes along the laser pulse propagation direction perpendicularly to the target surface. In the case of this spatial resolution the convergence within 5% precision is obtained even for such a low number of particles of each type per cell as 8.

THE DYNAMICS OF THE ELECTRON SPIN PRECESSION IN THE LASER WAKEFIELD ACCELERATION

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This work is aimed to study the polarization dynamics of an electron accelerating in a plasma wake wave exited by a short intense laser pulse. Thomas–Bargman–Michel–Telegdi equations [1] are used to derive a set of coupled equations for the precession of the spin $\mathbf{s} = \{s_r, s_\phi, s_z\}$ of a single electron in the laser wakefield acceleration:

$$\frac{ds_r}{d\zeta} = \frac{1}{u_z}\left(a + \frac{1}{\gamma}\right)\frac{d\Phi}{d\rho}s_z + s_\phi\frac{d\phi}{d\zeta};\ \frac{ds_\phi}{d\zeta} = -\frac{s_r}{u_z}\frac{d\phi}{d\zeta};$$

$$\frac{ds_z}{d\zeta} = -\frac{1}{u_z}\left(a + \frac{1}{\gamma}\right)\frac{d\Phi}{d\rho}s_r,$$

where variables comoving with the laser pulse are $\xi = k_{p0}z - \tau$, $\zeta = k_{p0}z$, $\rho = k_{p0}\mathbf{r}_\perp$, $k_{p0} = \omega_{p0}/c$ and a is the anomalous magnetic moment of the electron, τ is the time normalized to the inverse of the plasma frequency $\omega_{p0} = \sqrt{4\pi e^2 n_0/m_e}$, with e and m_e being the electron charge and mass, n_0 is the plasma density, Φ is the wakefield potential [2]. The electron velocity $\mathbf{u} = \{d\rho_x/d\tau, d\rho_y/d\tau, d\zeta/d\tau\}$ is connected with the dimensionless electron momentum $\mathbf{q}$ by the relation $\mathbf{u} = \mathbf{q}/\gamma$ and the trajectory of the electron can be obtained from the following equations:

$$\frac{dq_z}{d\zeta} = \frac{1}{u_z}\cdot\frac{\partial\Phi}{\partial\xi};\ \frac{dq_x}{d\zeta} = \frac{1}{u_z}\cdot\frac{\partial\Phi}{\partial\rho}\cdot\frac{\rho_x}{\rho};\ \frac{dq_y}{d\zeta} = \frac{1}{u_z}\cdot\frac{\partial\Phi}{\partial\rho}\cdot\frac{\rho_y}{\rho},$$

$$\frac{d\xi}{d\zeta} = \frac{u_z - 1}{u_z};\ \frac{d\rho_x}{d\zeta} = \frac{q_x}{q_z};\ \frac{d\rho_y}{d\zeta} = \frac{q_y}{q_z}.$$

In this work, on the base of obtained equations the scheme for numerical modeling of the selfconsistent spin dynamics of a single electron during the acceleration in plasma wakefields is developed and testing results of calculations for the case of uniform accelerating fields are in agreement with [3].

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TRAPPING OF ELECTRONS FROM THE ELECTRON BUNCH IN A WAKE WAVE

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The two-dimensional problem of trapping of electrons by the wakefield from the injected electron bunch has been studied analytically for an arbitrary ratio of the bunch dimensions to the characteristic dimensions of the wake wave generated in a plasma channel by a short laser pulse. The electrons are injected into the vicinity of the maximum of the wakefield potential with a velocity lower than the phase velocity of the wake wave. The process of the formation of a compact electron bunch in the trapping region due to the cutting out of electrons from the injected bunch has been considered. The parameters of the injection region in which the electrons are trapped and then accelerated by the wake wave have been determined. Formulas have been derived that allows one to accurately estimate the length of the trapped electron bunch and the number of electrons in it. It is shown that the influence of the transverse dimensions of the injected bunch on the length of the trapped electron bunch in the accelerating stage and its energy spread after acceleration is as important as the influence of its longitudinal size, because both of them can make comparable contributions to the length of the trapped electron bunch [1].

When a long wide electron bunch is injected into the wakefield, its dimensions do not enter into the formula for the length of the trapped bunch. In this case the length of the bunch is determined by the dimensions of the injection region, rather than by those of the injected bunch. The dimensions of the injection region depend on the electron injection energy.

Thus, the length of the electron bunch in the accelerating stage can be controlled by varying the value of the injection energy.

The parameters (the energy spread, emittance, and spatial dimensions) of the accelerated electron bunches formed in the course of electron trapping by the wake wave from injected electron bunches with different ratios between their spatial dimensions and the characteristic dimensions of the wakefield have been compared by means of numerical simulations. It is shown that the mechanism of cutting out electrons from the injected electron bunch allows obtain bunches of accelerated electrons with energies of ˜1 GeV, transverse emittances of 1–3 mm mrad, and relative energy spreads of several tenths of a percent.

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PARAMETRIC WAVES EXCITATION IN RELATIVISTIC LASER–PLASMA INTERACTIONS FOR ELECTRON ACCELERATION

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Plasma created by femtosecond laser pulse of high intensity can be used as the brilliant source of high energy electrons, ions and X- or γ-rays. In most cases, laser pulses with high contrast are used for acceleration particles. But, it has been shown, that changing parameters of pre-plasma layer on the surface of the target can significantly increase electron energies [1]. In this work we present the results of the experimental and numerical studies of the abnormally hot electron generation mechanisms in the case of long scale pre-plasma layer subcritical density.

In our experiments we used Ti:Sapphire laser system (p-polarized, $\lambda =$ 800 nm, $\nu_{\text{pulses}} = 10$ Hz, $E_{\max} = 40$ mJ, $\tau_{\min} = 45 \pm 5$ fs and $I_{\max} = 5 \times 10^{18}$ W/cm^2, ASE level – 10^{-8}). For creation controlled long and dense pre-plasma layer we used Nd:YAG laser ($\lambda = 532$ nm, $E = 30$ mJ, $\tau = 6$ ns, $I = 10^{12}$ W/cm^2) locked with Ti:Sapphire laser system. Were performed optical and γ-ray plasma diagnostics at different delays between the pulses and the focal positions of the main pulse. We observed several laser-plasma interactions regimes. In some of them, average energies of

hot electrons increases more than 7 times from 330 keV in the case of clear Ti:Sa pulse (ponderomotive acceleration) up to 2.4 MeV with artificial pre-pulse. Moreover, there is a strong correlation between the γ-ray yield and three-halves harmonic ($3\omega_0/2$) generation, it indicates the parametric processes participation in electron acceleration.

For clarification of the electron acceleration mechanisms numerical simulations were done using fully relativistic 3D3V PIC code Mandor (in 2D3V regime). A laser pulse (p-polarized, $\lambda = 1$ μm, $\tau = 50$ fs, $I = 10^{18}$ W/cm^2) was focused onto the targets with different pre-plasma layer parameters (corresponding to the experiments). The typical simulation box size was 90×15 μm^2 with periodic boundaries and spatial resolution of $\lambda/100$. Simulation showed that relativistic self-focusing, parametric processes, wave-breaking, stochastic heating, its combinations and variations, define the abnormally hot electron generation.

The work is supported by the RFBR (grant # 14-02-31871).

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DEVELOPING OF SUPERCONDUCTING NIOBIUM RESONATORS FOR ACCELERATING DEVICES

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Decision of scientific communities concerning building of the modern particle accelerators (XFEL [1], International Linear Collider (ILC) [2], as a number of smaller projects) create a demand for accelerating elements — superconducting high-frequency niobium resonators. The manufacturing process of a modern microwave resonator is an extremely complex task that requires highly specialized expensive equipment and the participation of specialists from various fields of science.

As part of the JINR project of the International Linear Collider five scientific organizations from Belarus joined their efforts to create experimental models of single-cell 1,3 GHz microwave niobium resonators in accordance with the requirements of the ILC project [3], [4]. The work package includes mathematical modelling of part geometry, manufacturing half-cells according to the reference profile by liquid impact forging, mechanical and chemical treatment of the blanks and the resonators, electron beam welding of units, 'warm' and 'cold' RF testing of resonators.

Electron beam welding, due to the ability to precisely control the energy density in the heating spot and maintain the original purity of the weld metal at the level of the base metal, is the only possible way of preparing the compounds of products made from ultrapure niobium for microwave cavities. In this paper we examine the relationship of welding parameters with the surface morphology, geometric characteristics of penetration zone of niobium, structure and mechanical properties of the weld metal and heat affected zone, the superconducting characteristics of the material after joining of welds components of microwave resonators. The paper presents the results of testing of the RF 1,3 GHz single-cell niobium cavities made in the PTI NAS of Belarus.

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WARM SOLID MATTER ISOCHORICALLY HEATED BY LASER-GENERATED RELATIVISTIC ELECTRONS

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The warm dense matter, generated due to the interaction of high contrast sub-PW laser pulses with solid matter of reduced dimensions, is investigated experimentally. During the interaction a considerable fraction of the laser energy is converted to relativistic electrons accelerated to MeV energies. These energetic electrons subsequently flood the target and heat up the remaining bulk electrons due to collisions and strong return currents on the time scale of picoseconds. Additionally, for the targets with reduced

cross dimensions, such as thin wires, strong electrostatic sheath fields confine the electrons to the target which efficiently and homogeneously heat it to high energy densities.

The experiment was set up at PHELIX facility providing high-contrast 0.5–1 ps laser pulses of ∼200 J energies. The laser was focused to a 4 μm spot at the tip of 50 μm Ti wires at 22.5° to the wire axis. To estimate the energy distribution of the heating electron flow, the bremstrahlung spectra was measured in the range of tens to hundreds keV. The temperature of the matter was measured by means of high-resolution X-ray spectroscopy with spatial resolution down to 20 μm along the wire axis, and accordingly the electron beam direction. It is shown, that at 5×10^{20} W/cm^2 laser intensity the electrons propagated up to 800 μm deep into the Ti wire. The value is below the calculated stopping range of the energetic electrons in solid Ti, showing the effect of Ohmic barrier due to the large return currents neutralizing the forward fast electron current.

The shape of TiK$_\alpha$ doublet spectral line was analyzed by comparison to the simulation data obtained using collisional-radiative hybrid-structure SCRAM code. The spatial distribution of He$_\alpha$ emission, registered together with TiK$_\alpha$ allowed to distinguish the area of the target heated directly by the laser impact from the deeper one heated by relativistic electrons only. It is proven that the solid Ti was isochorically heated by the electrons up to 50 eV temperatures. The work is partially supported by Russian Foundation for Basic Research (grant No 14-29-06099) and by RAS Program for Fundamental Research No 13.

NEW METHOD OF THE POLYMERIC MATERIAL PROPERTIES EXPERIMENTAL IVESTIGATION UNDER POWERFULL ENEGRY FLUX IMPACT

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Investigation of the polymeric material properties under powerfull enegry flux impact is relevant as for basic research (mathematical modeling of polymeric materials behavior in extreme conditions, testing the state equations), as for practical applications (for testing of protective coatings for space research and laboratory facilities). A lot of experiments for

investigating mechanical properties of different polymeric materials, and shock waves impact to them have been carried out as yet Experimental results often contradicted preliminary calculations. This fact demonstrates that presented problem was not researched properly enough. It should be noted that PMMA and polystyrene impact adiabat are well known [1], but there not enough data on destruction mechanisms of epoxy resins, PMMA, polystyrene and other polymers in the literature. In particular, the study of the process of the destruction of polystyrene and PMMA under the influence of the shock wave demonstrated difference in the spatial position of their destruction area [2, 3] in spite of the closeness of the many physical and technical parameters of these two polymers. This paper presents the results of experimental studies of the interaction of polymeric materials with a relativistic electron beam produced by a high-current electron accelerator Calamary. Calamary facility provide a wide range of electron beam parameters: diameter — 10–15 mm, the voltage on the diode up to 300 kV, the current through the diode up to 30 kA. New method of beam-target interaction area measurement was developed. The original method for the mechanical kick impulse measuring based on piezoelectric vibration sensor was presented. The dependence of the kick impulse from the power flux was obtained. This work was supported by the grant of RFBR 15-02-03544-a.

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2D SIMULATIONS OF THE DYNAMICS AND FRACTURE OF METAL IN THE ENERGY RELEASE AREA OF THE HIGH-CURRENT ELECTRON BEAM

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Metal behavior under the high-current electron irradiation [1] is an example of complex problem. Intensive energy release transfers the medium into an extreme state with high values of pressure and temperature. Leaving this state is accompanied by a number of dynamical processes: propagation of compression and release waves [2], fracture in solid state due to generation and growth of voids [3], melting and fracture of melt due to cavitation [4], evolution of the liquid-vapor two-phase medium, and frag-

mentation of melt on drops [5]. In present report, we pay attention to the evolution of the molten state of metal and to the processes of cavitation, evaporation and fracture of this state. We develop the continuous model of fracture. The model and its parameters are verified, at first, by comparison with the results of our molecular dynamics (MD) simulations, which are performed with the use of LAMMPS MD simulator [6]. Strength of initially uniform melts of aluminum, copper, iron and lead is calculated for a wide range of strain rates and temperatures. Also, we present a two-dimensional version of the mathematical model of the dynamic fracture of metal melt. The 2D model is necessary for description of the action of narrow-focused electron beams. Fracture of metals in molten state in the energy release area of the electron beam is numerically simulated; and the spatial distribution of the drops size is investigated.

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AHARONOV–BOHM EFFECT AND QUANTUM ELECTRODYNAMICS BACKGROUND

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Although the paper by Aharonov and Bohm was published more than 50 years ago,new aspects of the Aharonov-Bohm (AB) effect [1] attract great attention up to now [2]. The vector potential influence on particle motion ("effect without a force") was experimentally confirmed (e.g., A.Tonomura and F. Nori [3]). Most studies, including experimental researches, are devoted to the magnetic AB effect. However, in recent years the interest in the electric AB effect has significantly increased [4]. However, the elec-

tric AB effect contradicts the gauge invariance requirement for the scalar and longitudinal part of the vector potentials. Possible solution of this problem in quantum electrodynamics (QED) is based on the concept that only averaged values of operators can be observable. This concept opens the opportunity to consider the d'Alembert equations $\mathrm{D}\hat{A}^{\mu} = 4\pi\hat{j}^{\mu}$ for the operator of the four-vector potential $\hat{A}^{\mu}$ as the background of QED. Here $\hat{j}^{\mu} \equiv (\hat{\rho}, \hat{\mathbf{j}}/c)$ is the four-vector of the charge current and D is the d'Alembert operator $\mathrm{D} \equiv \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 \equiv \partial_{\mu}\partial^{\mu}$. To satisfy Maxwell equations for average fields the Lorenz relation should be valid only for averages values $\partial_{\mu}\langle\hat{A}^{\mu}\rangle = 0$ of the four-vector potential. The observable values of fields $\langle\mathbf{E}\rangle$ and $\langle\mathbf{H}\rangle$ are defined via average values of the potentials. In this formulation of QED the Maxwell equations for the field operators are not fulfilled. Accepting this background one can assume that the free quanta of the longitudinal and scalar potentials can exist and can be observable (at least in principle), whereas the photons of electromagnetic field are always transversal, as follows from the Maxwell equations for the averages fields in vacuum. In this way, we arrive at the statement that Maxwell equations for average fields do not provide the overall description of the electromagnetic field properties, but constitute only the fundamental part of a general description. This background provides the validity of all known QED results and additionally gives the basis for explaining of the recent data on the electric AB effect.

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CALCULATE THE PRESSURE OF LASER PULSES ON THE SURFACE OF SODIUM CHLORIDE

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Earlier in [1] studied the dependence of the critical electric field intensity (laser intensity) of the laser pulse duration in the case of radiation damage of sodium chloride. For further work on the analysis of very rapid destruction of the surface of an ionic crystal have been used data relating to the ablative surface area of destruction of sodium chloride. Because ablation is characterized by definite regularities, the calculated values of

ablation pressure can be used to analyze the dependence of the damage threshold of sodium chloride on the pulse duration in the selected range. In this paper, we calculated ablation pressure p_a by different formulas.

1. Use the formula given in [2]:
$p_a(kb) = 4.8 \cdot 10^{-4} I^{1/2} (W/cm^2)$, (1)
where I - intensity of the laser radiation.
2. Do the calculations for scaling [3]:
$p_a(Mb) = 12(I/10^{14}, W/cm^2)^{2/3} \cdot (\lambda, micron)^{-2/3}$ (2)
3. Use the formula discussed in [4]:
$p_a(kb) = 2.6 \cdot 10^{-4} I^{1/2} (W/cm^2)$. (3)

A value $p_a = 3\ Mb$ is achieved: by (1) with $I = 3.6 \cdot 10^{13}\ (W/cm^2)$, according to (2)-when $I = 1.5 \cdot 10^{13}\ (W/cm^2)$, according to (3)-when $I = 2.0 \cdot 10^{13}\ (W/cm^2)$. This high pressure is of great interest, since p_a more than 1 Mb on the surface of sodium chloride may occur insulator transition in metallic state [5, 6].

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EVALUATION OF SODIUM CHLORIDE DAMAGE THRESHOLD LASER PULSES NANOSECOND AND PICOSECOND

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Based on the experimental data given in [1, 2], previously we analyzed the dependence of the breakdown threshold of the laser (the critical field

strength) of sodium chloride by laser radiation pulse duration in the femtosecond range. On the example of ionic crystals and fused quartz revealed that possible approximation damage threshold of destruction several direct with different angular coefficient [3, 4]. In this paper, has been tasked to a more complete assessment of radiation resistance of sodium chloride laser pulses of nanosecond and picosecond. We used some of the experimental data on the range of the laser pulse duration [5, 6]. Calculation and analysis of the results were performed for laser pulses of $10ns - 10ps$. Also considered a number of possible mechanisms for the destruction of an optically transparent solids by laser pulses of nanosecond and picosecond. Particular attention is paid to the destruction of ionic crystals avalanche of electrons due to impact ionization [7]. Irradiation of the solid material of high energy laser pulses can result in the removal of material from the surface of the material. This phenomenon, called laser ablation is often the main mechanism for the destruction of ionic crystals in the picosecond and femtosecond range. Because ablation is characterized by definite regularities, it can be used to analyze the damage thresholds of sodium chloride in the picosecond laser pulse.

This work was supported in the framework of the base part of the Russian DES government task KBSU for years 2014-2016 (Project $2014/54 - 2228$).

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THE OPTICAL STRENGTH OF THE GLASS NANOCOMPOSITES BY LASER ABLATION STUDIES

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Theoretic and experimental studies of the optical strength of the nanocomposite materials (glass, polymer, fiber optic elements, and so on) in [1-4] have been fulfilled to account for the influence of material physical factors on the optical strength. The results of our experiments in [1, 2] with using Weibull-Gnedenko statistics related to a single irradiation of the sample, can be used to predict the optical strength R of the sample when one is interacted with pulse laser radiation. If the repetition rate of the laser pulses is equal to f, then after time t the total number of pulses is equal to $N = ft$, we obtain the optical strength of the sample at time t:

$$R(F,t) = e^{-ln2\frac{F^m}{F^m_{0.5}}ft}.$$

The parameters $F_{0.5}$ and m are determined from the experimental results and the repetition rate of laser pulses f is an input parameter. Thus, the use Weibull-Gnedenko statistics allows us to predict the polymer nanocomposites optical strength during the time t pulsed radiation with a pulse repetition frequency f (in our case $f = 10$ Hz).

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THE LASER ABLATION STUDIES OF THE GLASS NANO COMPOSITES WITH THE DIFFERENT OPTICAL PROPERTIES

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The glass nano composites laser ablation destruction parameters dependencies on the nanofilm refractive index and light transmittance values have been studied in this work as a continuer of our earlier works [1–3].

The samples were the glass plate with dimensions of $50 \times 50 \times 4$ mm. Film creating solution has one SiO_2 or TiO_2 or two oxides –TiO_2 + CdO, CuO or SnO with the 2 mass.% of the film creating oxides in sol total concentration that is equal to 5%. The glass plate extraction velocity from the sol was about 3.8 mm/s. The samples transmittance values were recorded by FSD 8 type micro spectrometer and the composite average value T_{mid} was calculated for every sample in the visible range of the spectrum. The film refractive index n and its thickness h have been measured by Uvisel 2 spectral ellipsometer.

The laser ablation destruction threshold energy density values measurements have been fulfilled for these samples at the laboratory laser ablation station created on the basis of experimental setup in [1, 2]. The YAG-Nd laser generates pulses at the 1064 nm wavelength with time duration of 20 ns and pulse energy up to 150 mJ (F_{bn}) and 300 μs with energy 1.2 J (F_{bm}), accordingly.

The generated plot of the probability was determined by the ratio of the shots number with breakdown and the plasma plume emission presence to the general shots number for the given sample due to the laser ablation destruction probable character. The threshold energy density F_b values have been taken from these dependence curves for the equal experimental condition and the breakdown probability $P = 0.5$ [2].

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ANALYSIS OF OPTICAL FIBER DESTRUCTION CAUSED BY LASER SUPPORTED DETONATION

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There are two modes of propagated damage caused by laser radiation in silica-based optical fibers. This work presents the investigation of detonation-like mode. The propagation velocity of a plasma front is two orders of magnitude greater than for a fiber fuse effect (combustion mode). This mode is new object of laser destruction of silica-based optical fibers. Such bulk damage becomes significant due to progress in fiber optical application. Optical fiber and enough long laser pulse let us obtain laser damage propagated near hundred fiber core diameters during pulse. The use of optical fibers provides the important advantage. It allows supply the same form of energy deposition in the every cross section of optical fiber. Tested regime demonstrates near constant velocities during 200 ns in the range of laser intensity 2–4.5 GW/cm^2. After plasma propagation, irreversible damages are obtained in the optical fiber. We have investigated the damage by a scanning electron microscope. Melted and crushability zones have been visualized and measured.

DIRECT LASER INITIATION OF OPEN SECONDARY EXPLOSIVES

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The use of laser pulse instead of electric heating for initiation of explosives is considered as a promising alternative, which is insensitive to external electromagnetic influences. In addition, short laser pulses can significantly reduce and optimize the ignition-period of the explosion. Therefore, the laser radiation impact on energetic materials is in recent years the subject of comprehensive studies in many scientific centers (see, for example, reviews in publications: I.G. Assovskiy, Physics of combustion and interior ballistics. Moscow: Nauka, 2005; V. I. Tarjanov "Pre-explosion phenomena in rapid initiation of high explosives (review)", Combustion, Explosion and Shock Waves, 2003, V. 39, No.6.). The goal of this paper is a theoretical and experimental study of the mechanism of initiation of explosion in secondary explosives (SE) by short laser pulse. Laser initia-

tion of SE is much more difficult in comparison with initiation of primary explosives. Typically using of some special methods is requested to realize laser initiation of SE: putting of explosive in closed volume and using of porous SE. In this paper we consider interaction of laser pulse with open surface of non-porous SE. Only pure chemical methods as well as metallic additives were used to control the light sensitivity of SE. Implementation of the method of laser initiation is reduced to the optimization of composition and molecular structure of the explosives, thermo-mechanical properties of metallic additives, along with the optimization of the laser pulse (its duration, energy density and wavelength), taking into account the great variety of secondary explosives and conditions for their functioning, as well as the laser beam diameter, the beam divergence and dynamics of the pulse power variation in time.

THE THz SCANNING FOR THE MEASUREMENT OF THE DENSITY CHANGE IN STRAINED FOAMS

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Introduction. This paper is devoted to the development of the technique for the estimation of a distribution of mechanical stress on the strained specimen based on terahertz absorption data.This hypothesis is based on the relation between density of the stressed material and absorption of THz radiation. The THz technology is strongly demand in a large variety of fields, ranging from the fundamental sciences such as biochemical spectroscopy, astronomy, and condensed-matter physics to practical applications such as high-capacity communication, medicine, agriculture, and security [1, 2].

General part. The deformation of an object is generally accompanied by the change of its density. However, the density depends on a stress. The polymeric foam was chosen for the study of its mechanical properties and absorption ability of the THz radiation. A combination of the dependence of the density and stress with the approximation of the relative absorption-strain plot gives us a relation between absorption of the THz beam and intensity stress tensor. Using the experimental set up developed by NeTHIS the authors estimated the stress distribution near the holes with different diameters in stressed polymeric foams. The specimen

was fixed between two Teflon plates and compressed by four screws.

Conclusion. As a result of this work authors propose a new way for the estimation of a stress distribution in porous non-metals bodies based on the absorption of the THz beam. The results of the mechanical testing and numerical simulation show the good qualitative agreement and high efficiency of the THZ based experimental technique. The THz based methods can be considered as a promising way for the obtaining of the quantitative information about the stress-strain state of the Thz transparent bodies.

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EFFECTIVE CREATION OF POSITRONS IN MATTER UNDER HIGH ELECTRIC FIELD OF INTENSE LASER PULSE: TO EXPLANATION OF BALL LIGHTNING NATURE

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Recently, very efficient creation of positrons was demonstrated by irradiating in vacuum a thin ($\sim$1 mm) gold target by short ($\sim$1 ps) and highly intense ($\sim 10^{20}$ W/cm^2) laser pulse [1]. As observed, positrons appeared as a flying forward restricted beam with high their density ($\sim 10^{16}$ cm^{-3}). Positrons were produced in the process of electron-positron pair creation that is a last stage of known (in high energy physics) processes, which occur in matter due to very high electric field (of laser pulse, in this case). First, due to very high electric field the electron appearance, heating and multiplication (by ionization of matter particles) take place. Then very hot electrons effectively produce bremsstrahlung (gamma quanta with MeV energy) at their retardation in the electric field of atomic nucleus. At last, these gamma quanta also effectively (in the electric field of atomic nucleus) create electron-positron pairs, where electron and positron fly away in the opposite directions. Recently, efficient positron creation was revealed in thunderclouds with space telescope Fermi by registration a radiation of electron-positron annihilations. This fact is confirmed by mountainous station observations that discover also the appearance in thunderclouds of electrons and gamma quanta with MeV energies [2]. Their creation is due

to existence in thunderclouds of high electric fields (up to 200 MV), which generate powerful electrical discharges (lightning with up to 10^{20} high energy electrons), that often leads to appearance of mysterious ball lightning. An assumption that ball lightning is bunch of many (up to 10^{17}) next to created positrons lets explain all its properties. The possibility of positron aggregation is substantiated by existence of dark matter (in all ambient space) and understanding created positrons as a wirls shaped from dark matter.

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THE DESIGN, CONSTRUCTION AND TESTING OF TASD (TOTALLY ACTIVE SCINTILLATOR DETECTOR)

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Under the project AIDA Institute of Nuclear Research (TASD) are design and testing TASD. This document reports on the design of TASD detector prototype and outlines requirements for a test beam at CERN to test these, tentatively planned on the H8 beamline in the North Area, which is equipped with a large aperture magnet.

The TASD detector consists of 50 modules of plastic scintillators. Each module is instrumented with one X and one Y plane, with 90 scintillator bars per plane. The bar width, height and length are 1.0 cm, 0.7 cm and 90 cm respectively. The distance between modules can be varied from 0 to 2.5 cm. Other components such as active detectors or passive sheets of material can be inserted in these 2.5 cm gaps if required. The full detector depth can therefore be varied from 75 cm to 200 cm and in its compact form, it is 1 m^3 in volume.

This document reports the results of design of TASD, measurements results of elements, that included in the prototype elements (measurement of cross-currents, the light yield of scintillators, the characteristics of photodiodes).

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COMPARISION OF CATHODOLUMINESCENCE AND GAMMA LUMINESCENCE DECAY TIMES OF SCINTILLATORS

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The decay times of cathodoluminescence of LSO and LYSO scintillators had been measured using CLAVI facility, upgraded for decay time measurement by DMR-4 prism monochromator, FEU-62 PMT tube and Tektronix digital oscilloscope with bandwidth 300 MHz. Time resolution of the system is approx. 15 ns. It was found that the decay times of all crystals are equal to each other. The value of all decay times is 50 ± 7 ns. This result was compared with the decay times of luminescence of this scintillators under the action of gamma irradiation. Gamma luminescence decay times had been taken from literature. The result is the decay times of gamma luminescence and cathodoluminescence are equal within the measurement errors. This results proves the possibility of the cathodoluminescence methode usage for scintillator's decay times measuring.

The work was financially supported by the Russian Science Foundation (proj. 14-22-00273)

EVALUATION OF THE SENSITIVITY OF THE GAS-DISCHARGE GAMMA-COUNTERS TO THE CONCOMITANT NEUTRON RADIATION

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In the fields of gamma-neutron radiation accuracy measurement of gamma-ray doses depends on their sensitivity to concomitant neutron radiation which is registered by the counter recoil nuclei and nuclear reactions products occurring in the counter case and gas. In this connection, verification results of gamma-dosimetry on the with isotope cobalt or cesium sources are not always adequate to measurement results in real gamma-neutron fields. The studies were conducted in standard fields of PRIZ-M reactor gamma-neutron radiation and in the field of standard cobalt gamma-ray source. The absorbed dose of gamma-ray in standard field was measured at the metrological certification of the installation with a set of ionization chambers out of the composition of the military standard VE-19PDN-2 at an error of 9.5%. The objects of investigation are gas-discharge counters SBM-20. The coefficients of sensitivity to gamma-rays are determined experimentally, their values are equal to the ratio of counter indication to the absorbed dose of gamma-rays in a standard tissue. By the same algorithm the values of sensitivity coefficients to gamma-ray of Co^{60} standard source have been determined. The table data prove, that the sensitivity coefficients of gamma-dosimeters with SBM-20 counter at PRIZ-M reactor is 1.23 larger as compared to Co^{60} source, due to the effect of the concomitant neutrons on their indications. The error due to the neutrons effect can be significantly reduced or eliminated completely, if gamma-dosimeters calibrated in the field of gamma-neutron radiation, adequate spectral and dose characteristics to radiation fields in which they are used. To solve this problem at PRIZ-M reactor the model field of gamma-neutron radiation was created by variety of materials, transforming the radiation parameters to the desired values. The criterions of similarity are the energy spectra of neutrons and ratio of neutron and gamma-ray doses in real radiation field. Radiation parameters in a model field were investigated by the calculated and experimental methods by means using ROZ-6.5 program. Research results indicate that the error of measurement gamma-ray dose in real gamma-neutron fields is two times lower at the dosimeter calibration in model field than in a cobalt source.

MCP BASED DETECTORS FOR REGISTRATION OF PARAMETERS OF X-RAY, GAMMA AND NEUTRON RADIATION OF HIGH TEMPERATURE PLASMA

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Fast detectors, based on microchannel plates (MCPs), have been developed for dynamic measurements of high-temperature plasma at high-power laser facilities. TSDI43 detectors are designed to implement TOF method of measuring the ion temperature of neutron sources. TSDI45 is intended for use in the hard X-ray spectrometers. TRPE8 detector is designed to obtain images in soft X-ray radiation with nanosecond frame duration. The report presents the results of studies the characteristics of detectors such as temporal and spatial resolution, linear currents and the spectral sensitivity.

PULSED NEUTRON GENERATORS OF VNIIA ON THE BASIS OF THE SEALED CHAMBERS OF PLASMA FOCUS DESIGN WITH D–D AND D–T FILLINGS

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Development of neutron generators using plasma focus (PF) chambers is being conducted in VNIIA during more than 25 years. PF is source of soft and hard X-rays and neutrons 2.5 MeV (D-D) or 14 MeV (D-T). Pulses of X-rays and neutrons have a duration of about several tens of nanoseconds, which defines the scope of such generators—the study of ultrafast processes.

VNIIA has developed a series of pulse neutron generators covering the range of outputs (10^7–10^{12}) n/pulse with resources on the order of 10^3–10^4 switches, depending on purposes. Generators have weights in the range 30–700 kg, which allows to refer them to the class of transportable generators.

Generators include sealed PF chambers, whose manufacture was mastered by VNIIA vacuum tube production plant. A number of optimized PF chambers, designed for use in generators with a certain yield of neu-

trons has been developed. The use of gas generator based on gas absorber of hydrogen isotopes, enabled to increase the self-life and resource of PF chambers. Currently, the PF chambers withstand up to 1000 switches and have the safety of not less than 5 years. Using a generator with a gas heater, significantly increased security of PF chambers, because deuterium-tritium mixture is released only during work, other times it is in a bound state in the working element of the gas generator.

MULTICHANNEL WIDERANGE SPECTROMETER OF PULSED X-RAY RADIATION (TSRI1)

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Three types of high-speed detectors TDRI5, TDRI6, TDRI7 have been developed for soft x-ray fluxes detection with pulse duration from ∼1 to 20 ns. The detectors can be used under pressure of $< 1 \cdot 10^{-4}$ Torr at vacuum chambers of high-power laser and electrophysical facilities. The x-ray cathode of TDRI5 and TDRI7 is thin, less than 3 μm metal layer of Ni, Al or Au deposited over substrate. TDRI6 is based on open-type single 8-mm diameter MCP plate with chrome deposition (TDRI6-01 is dual-MCP modification). Detectors are sensitive to x-ray photons with energy of 0.05 to 10 keV. The time resolution of detectors, determined as pulse duration on 50% level, was measured on x-ray pulse installation based on 10 mJ femtosecond laser. $\tau_{\frac{1}{2}}$ for TDRI5 and TDRI6 is less than 0.2 ns, $\tau_{\frac{1}{2}}$ for TDRI7 is less than 0.5 ns. A sensitivity of detectors is more than 10^{-4} A/W for all modifications and can be adjusted by MCP voltage on TDRI6 or by using of grid dampers on TDRI5 or TDRI7. Maximum levels of linear pulse current are 0.5 A for TDRI6, 2.5A for TDRI7 and 4 A for TDRI5 with supply voltage under 2.5 kV.

VACUUM X-RAY DETECTORS FOR DIAGNOSTICS OF FAST PROCESSES IN PLASMA

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Three types of high-speed detectors TDRI5, TDRI6, TDRI7 have been developed for soft x-ray fluxes detection with pulse duration from ∼1 to 20 ns. The detectors can be used under pressure of $< 1 \cdot 10^{-4}$ Torr at vacuum chambers of high-power laser and electrophysical facilities. The x-ray cathode of TDRI5 and TDRI7 is thin, less than 3 μm metal layer of Ni, Al or Au deposited over substrate. TDRI6 is based on open-type single 8 mm diameter MCP plate with chrome deposition (TDRI6-01 is dual-MCP modification). Detectors are sensitive to x-ray photons with energy of 0.05 to 10 keV. The time resolution of detectors, determined as pulse duration on 1/2 level, was measured on x-ray pulse installation based on 10 mJ femtosecond laser. $\tau_{\frac{1}{2}}$ for TDRI5 and TDRI6 is less than 0.2 ns, $\tau_{1/2}$ for TDRI7 is less than 0.5 ns. A sensitivity of detectors is more than 10^{-4} A/W for all modifications and can be adjusted by MCP voltage on TDRI6 or by using of grid dampers on TDRI5 or TDRI7. Maximum levels of linear pulse current are 0.5 A for TDRI6, 2.5 A for TDRI7 and 4 A for TDRI5 with supply voltage under 2.5 kV.

KRYPTON SINGLE AND DOUBLE K-VACANCIES ENERGIES AND TWO-ELECTRON PHOTOIONIZATION CROSS SECTION DETERMINATION BY MEANS OF PROPORTIONAL COUNTER

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Experiment has been carried out with Kr proportional counter exposed to characteristic X-ray. On the base of peak shape analysis the selection of events corresponding for candidates on two-electron photoionization has been done. Numerical calculations were done in the frame of Hartree–Fock [1] and distorted wave approximations [2].

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ON THE POSSIBILITY OF USING THE DEFORMATION DEFECTS IN ^{29}Si FOR CUBIT TECHNOLOGY

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Paramagnetic defects of new types are generated as a result of plastic deformation of isotopically enriched ^{29}Si. A correlation of temperature behavior of dislocation luminescence lines and the magnetic susceptibility was found experimentally. The electron paramagnetic resonance spectra (EPR) are anisotropic and have a considerable width (up to 1 kOe). Nonuniform broadening of EPR bands is determined by variations of internal magnetic field in the correlated defect clusters. The nuclear magnetic resonance (NMR) spectra of the deformed crystals are Pake doublets splitted by spin-spin nuclear interaction. The broadening of NMR spectra is caused by a dipole-dipole relaxation.

COMPLEXITY OF ELECTRONIC TRANSPORT IN THE IRRADIATED CRYSTALS OF ORGANIC QUANTUM "SPIN LIQUID" κ-$ET_2Cu_2(CN)_3$

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Single crystals of organic charge-transfer salt κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ (κ-CN), where BEDT-TTF is an organic single electron donor molecule -*bis*(ethylenedithio)tetrathiafulvalene), recently attracted considerable attention due to discovery of the mysterious state of matter - "spin liquid" state. The state demonstrates no spin order down to the lowest temperatures available to the experimentalists (10 mK and recently, lower) despite strong spin coupling interactions existing in the lattice of κ-CN (J = 250 K). It is speculated that the effect is explained on the basis of an ideal triangular spin lattice realized in the salt, which gives no favor to

any paired interaction, and strong quantum fluctuations persisting in the lattice.

In the presented work, samples of κ-CN of different quality were exposed to a range of X-Ray radiation doses (10^5–10^8 Gy). Resistivity measurements were performed at each step prior and after irradiation. We found that while in the dielectric mode (amb. pressure) the irradiation lead only to a slight depression of an activation gap, whereas in the superconductive mode ($p = 1.4$ kbar) the irradiation influence is dramatic. Fermi liquid ($R(T^2)$ is linear) region that normally precedes to T_c (critical temperature) is destroyed even by minor doses of radiation, T^* (pseudogap opening temperature) is transformed from a distinct peak to a broad bad resolved feature, T_c itself is broadened and shifted to lower temperatures or disappeared. The strong κ-CN sample dependence and uncalibrated X-Ray source did not allow us to track down the clear and quantitative dependence of the observed effects from the exposition doses and make conclusive remarks. Based on the hypothesis that the superconductive mechanism in the compound is a $d-wave$ both magnetic and non-magnetic scattering centers should damp superconductive state. However, observed strong influence of the implanted defects on Cooper pairing hints us the magnetic nature of the scattering centers. That is in the contrast with the literature data those claim the X-Ray implanted defects are non-magnetic for the other close related salts of κ-family: κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ & κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br. Our preliminary results revealed higher sensitivity of a superconductive state in κ-CN to radiative damage than in other κ-salts. The importance of these results dictates thorough and accurate measurements together with subsequent result interpretations those are planned in a nearest future.

SOME PROBLEMS OF WOBBLER SYSTEM APPLICATION FOR CYLINDRICAL TARGET IRRADIATION BY MEANS OF AN INTENSE HEAVY ION BEAM

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Heavy ion beam may be used for the matter extreme state creation [1], a forming beamline must satisfy to certain requirements on beam characteristics and focus position at the target. The original method of hollow ion beam formation—wobbler system—was proposed to deposit the beam energy at cylindrical target [2]. The disagreement of wobbler deflector

frequencies leads to undesirable violation of experiment requirements. In the paper presented the results of simulation are described that prove the effective energy losses and symmetry violation of the target irradiation due to frequency shift for fixed beamline geometry.

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DEVELOPMENT OF PERMANENT MAGNET QUADRUPOLE LENSES FOR PROTON MICROSCOPY EXPERIMENTAL FACILITIES

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One of the most effective methods to study of static and dynamic dense (up to 300 g/cm^2) objects is the method of high-energy proton radiography, allowing high spatial resolution and high contrast to investigate the density distribution in the object under study. Existing proton radiography facilities in USA [1] and in Russia [2, 3] clearly showed advantage of the proton radiography method compared to conventional X-ray methods, the study of dense objects, especially in dynamic experiments. The best spatial resolution of the proton radiography method was obtained in setups with increasing image of the object constructed by the scheme of the proton microscope [1–3]. Quadrupole lenses on permanent magnets (PMQ) with a high magnetic field gradient at small geometric dimensions are used create such facilities. The report is dedicated to the development of PMQ lenses for PUMA (ITEP, Moscow, Russia) and PRIOR prototype (GSI, Damstadt, Germany) facilities. In this work presents the description of the analytical, software and hardware to measure and tuning of magnetic field distribution in the PMQ. Presents the results of PRIOR PMQ magnetic field degradation caused by radiation damage by intense beam of protons in the SIS-18 accelerator.

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THE METHOD OF CALCULATION AND OPTIMIZATION OF THE ION-OPTICAL SCHEME OF THE PROTON MICROSCOPE

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The method of high-energy proton microscopy is widely used for investigate of dense static and dynamic objects. Numerical simulation of ion-optical scheme of proton microscopy facility is important task for the provide best spatial and density resolution of proton-radiographic images. The method based on principals of the matrix formalism [1] was developed for matching and optimization the ion-optical scheme. Method allows to find the optimal parameters of the ion-optical scheme. The developed tools and method is characterized in that allows to calculate scheme of the proton microscope for a wide range of input data, ie, for a wide range of energies of the proton beam and different configurations of quadrupole lenses used in the scheme. The method provides the best spatial resolution of proton-radiographic images with minimized chromatic aberration. Numerical simulation for existing and planned facilities (PUMA at ITEP (Russia) (Ep = 800 MeV) [3], new proton microscope scheme for Ep=300 MeV) was produced in frame of COSY Infinity environment [2]. In particular method can be used to matching of PRIOR [4] (Proton microscope for FAIR) (Germany).

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THEORETICAL AND EXPERIMENTAL STUDIES OF RADIATIVE AND GAS DYNAMIC PROPERTIES OF SUBSTANCES AT HIGH ENERGY DENSITY IN MATTER

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Mathematical modelling of radiative and gas-dynamic processes in substances at high energy density is carried out for experiments, where both laser and heavy ion beams are used. Important features of the theoretical model, known as the ion model (IM), which is used for quantum mechanical calculations of radiative opacity, are discussed. Reliability of (IM) results is tested with experiment, where measurements of X-pinch radiation energy yield for two exploding wire materials, NiCr and Alloy 188 were made. Theoretical estimations of radiative efficiency are compared with experimental results, and (IM) calculations agree well with the experimental data [1]. Subsequently, the theoretical approach was used for temperature diagnostics of CHO plasma target in combined laser - heavy ion beam experiments [2]. Joint radiative and gas-dynamic calculations are performed for comparison with experiment, where hohlraum radiation transmits through the CHO plasma target, and the share of absorbed radiation energy is compared with experiment [3]. Study of radiative properties of CHO plasma with little admixture of gold is carried out as well. Specific dependence of the Rosseland mean on plasma temperature is discussed for gold plasma.

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THE CREATION OF THE NEW SEGMENT "EMISSION SPECTROGRAMS" OF THE ATOMIC DATABASE SPECTR-W3

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The Spectr-W3 information-reference system was developed in 2001–2013 and realized as an online Web resource based on the factual atomic database Spectr-W3 (http://spectr-w3.snz.ru). The information accumulated in the Spectr-W3 atomic database contains about 450,000 records and includes the experimental and theoretical data on ionization potentials, energy levels, wavelengths, radiation transition probabilities, and oscillator strengths, and the parameters of analytical approximations of electron-collisional cross-sections and rates for atoms and ions. Those data were extracted from publications in physical journals, proceedings of the related conferences, special-purpose publications on atomic data, provided directly by authors and obtained in previous years by the Spectr-W3 project participants. The information is supplied with references to the original sources and comments, elucidating the details of experimental measurements or calculations. To date, the Spectr-W3 atomic database is still the largest factual database in the world, containing the information on spectral properties of multicharged ions. In 2014 the new stage in the development of the Spectr-W3 atomic database was started. The purpose of this stage is the creation of a new information segment of the Spectr-W3 database. This segment will contain information on emission X-ray spectrograms observed in various plasma sources. In the present time the software for this segment has been created for local version Spectr-CD of the database and has been tested. The set of the spectrograms obtained mainly in the laser-produced plasma was prepared. In 2015 the segment "Emission spectrograms" will be available in the Web-version of the database Spectr-W3. The work has been supported in part by the RFBR grant Nr. 14-07-00863-a.

THE GENERATION OF LOW-FREQUENCY RADIATION AND SURFACE WAVES UNDER THE ACTION ON THE CONDUCTOR THE FOCUSED LASER PULSE

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A theory of generation of electromagnetic radiation and surface waves in the terahertz frequency range is given for the case when focused by a cylindrical lens femtosecond laser pulse acts on the conductor. It is shown that ponderomotive force created by laser pulse leads to the excitation of nonlinear vortex currents in the skin layer of the conductor, which are the sources of both low-frequency radiation, emitted from the surface of the conductor into a vacuum, and the low-frequency surface waves propagating along the surface of the conductor. The field of low-frequency radiation arises from the parts of Fourier transform of the ponderomotive potential, for which the ratio of frequency module to the module of wave vector component along the surface of the conductor greater than the speed of light. The other parts of Fourier transform of the ponderomotive potential, for which this ratio is less than the speed of light, generate surface waves. The spectral and energy characteristics of low-frequency radiation and surface waves, as well as their spatiotemporal structure are investigated. It is shown that the spectrum of low-frequency radiation and surface waves has a wide bell shape maximum at frequencies close to the inverse the laser pulse duration. The total energies of low-frequency radiation and surface waves are calculated and their dependence on the laser pulse parameters and characteristics of the conducting medium and studied. It was found that at a fixed energy and duration of the laser pulse the maximum of the energy of low-frequency radiation and surface waves is achieved for tightly focused laser radiation. In the case of focusing of the radiation in the band with width of the order of the pulse length, and its length is much greater than the width, one can significantly increase the overall energy, as low-frequency radiation and surface waves, compared to their maximum values when focusing of the laser pulse in the spot with radius of the order of the pulse length. The increase is characterized by the order parameter of the ratio of the length of the band to the length of the pulse.

THEORETICAL AND EXPERIMENTAL STUDY OF INERTIAL GASES ADMIXTURES INFLUENCE ON THE HARD X-RAY EMISSION OF PLASMA FOCUS

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This paper studies the influence of inertial gases admixtures (Ar,Kr,Xe) to deuterium in plasma focus (PF) chambers. Experiments were realized on PF chambers with discharge currents 350 kA, 700 kA, 1000 kA. The measurement of the hard X-ray (HXR) emission were carried out by the scintillation detector SSDI-38 with time resolution 2.5 ns. Experiments shows the existence of optimum amount of inertial gases, which corresponds with the atomic number of added gas. On the optimum amount of inertial gas and deuterium in PF chamber the HXR yield rises up to 10 times in comparison with HXR yield only on deuterium filling. This work shows the dependence of HXR emission on PF device stored energy.

The mechanism of inertial gases admixtures influence that leads to rise of HXR yield has been discussed. The mechanism concern with different behavior of deuterium ions and ions of inertial gases during the pinch decay phase when the discharge current compression force has reduced. Inertial gas ions locates near the axis of the pinch and deuterium ions goes to the near plasma area. Local positive charge in plasma forms on this axis because of multiply charged ions of inertial gases. Then electrons gather to the axis area under the influence of the induced electromotive force during the pinch decay phase. HXR emission is generated after the electron beam interact with the anode target in PF chamber.

SET OF DEVICES FOR SIMULATION OF COMPLEX ACTION OF RADIATIONS AND PARTICLES FLUXES

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Forecasting of consequences of thermal and mechanical actions of radiations and particles fluxes (RPF) for composite constructions represents considerable interest [1, 2]. Usually thermal action accompanies mechanical action. Constructions accumulate heat at repeated RPF influences. Such accumulation can reduce construction strength durability to me-

chanical action. Thus researches of complex RPF action realized on a construction is almost important [3].

Carrying out experimental studies for direct and repeated RFP influence localized on large-scale construction is impossible or expensive in many cases. As rule settlement and experimental approach [2] is used. Realization of this approach demands creation of devices set for simultaneous modeling of thermal and mechanical RPF actions.

In present work the devices set is offered for reproduction of complex RPF These devices reproduce heatings (to one thousand degrees) and impulses of pressure (0.01–1 kPa s) having duration (0.05–300 μs). Various ways of generation of non-stationary thermal and mechanical loadings are used. Mechanical loadings are generated by an explosive detonation or electric explosion of a metal foil or a throwing of plates. Thermal fluxes are generated by the laser radiation or highest frequency radiation or heating elements or a stream of high-temperature gases.

Results of research of pulse loads action realized on composite three-layer samples are represented. Two external layers carry out protective functions (in particular it is the damping and heat-insulating functions. The third protected layer is carrier part of a studied design. The uneven temperature profile is done in these samples before reproduction of mechanical action. The received results allow us to draw important conclusions about efficiency of various variants of constructional protection designed from complex RPF action.

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NUMERICAL CODE FOR CALCULATION OF PARAMETERS OF MECHANICAL RADIATION ACTION ON THE HETEROGENEOUS SHEETINGS HAVING THE IRREGULAR DETERMINED STRUCTURE

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Protection of vehicle constructions against the ionizing radiation (IR) having quanta energy of 1–150 keV is an actual problem [1]. Progress of modern technologies of synthesis of the gradient heterogeneous materials containing a microspherical filler allows to create effective sheetings for protection against this type of radiation. Dispersions of parameters of a disperse filler by the sizes, a form and integrity are inevitable at making of constructions and their sheetings in uniform technological process. The deviation of spatial distribution of filler from the set gradient law takes place also. Existence of technological defects reduces protective characteristics of sheetings. Therefore development scientific and methodical technology is required to for forecasting of influence of technological deviations for parameters of mechanical IR action. The offered numerical code unites modeling of three groups of physical processes in a uniform settlement complex. There are transfer of radiation and energy absorbing [2] and quasistatic relaxation of the stress–deformation state localized in a heterogeneous cell [3] and wave processes [4] taking place at interaction of separate cells. Realization of these processes proceeding in the listed sequence leads to formation of mechanical IR action. Irregularities of structure are considered at all stages of this formation. It is realized at the level of an elementary cell for the first two stages. The irregularities which are available in distribution of particles clusters of filler in the binder are taken into account at the final stage. Results of calculations by means of the offered numerical code show essential influence (tens percent) of irregularities on parameters of mechanical IR action.

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PARAMETRICAL MODEL FOR THE ELEMENTARY CELL OF THE HETEROGENEOUS SHEETINGS HAVING THE IRREGULAR DETERMINED STRUCTURE

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The method of elementary cell [1, 2] is widely used for calculation of parameters of mechanical action of the ionizing radiation (IR). Now the representative set [3] of such cells is created. Usually uniform filler distribution is supposed at creation of elementary cells of heterogeneous materials. This assumption significantly simplifies a task. But the real heterogeneous sheetings (HS) have no periodic structure as a result of technological errors. Besides filler distribution uniformity doesn't take place in perspective gradient HS. In the present work the non-stationary model of an elementary cell is offered for the sheetings having the set of irregular structure. It is supposed [4] that tension relaxation taking place in a cell is quasistationary. Then only heat exchange between the HS components appears the reason of transitional processes being realized in a cell. The special attention is paid to the accounting of structural features of the multilayered microspherical fillers used in HS for protection from IR. Stability loss, destruction and irreversible microspheres collapse when IR energy is absorbed by a heterogeneous material are considered. As result of systematic calculations parameters of the tension-deformation condition of cell are received. These parameters are presented as function from dimensionless parameters of irregularities and the relation of time of IR energy absorbing to characteristic time of heat exchange realized in a cell. It is shown that the accounting of existence of structure irregularities which take place in practice leads to growth of tension in a cell for 20-30%. The received results will be used in multidimensional numerical models of formation of mechanical IR action localized on the HS.

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REFLECTIVITY AND IMAGING CAPABILITIES OF SPHERICALLY BENT CRYSTALS STUDIED BY RAY-TRACING SIMULATIONS

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Spherically bent crystals are widely used in focusing monochromators, spectrometers and other x-ray optical systems. In particular, they are used as dispersive elements in focusing spectrometers with spatial resolution. These spectrometers provide diagnostic of high energy density states of the matter including femtosecond relativistic laser plasma, plasma jets and shock waves in nanosecond laser plasma, etc. Plasma parameters are obtained via measurements of relative intensities of characteristic spectral emission lines for plasma multiply charged ions. The measured intensity of each spectral component is affected by an instrumental function determined by both a particular area on the crystal surface where this spectral line is reflected, and the crystal reflectivity function. The main goal of the work is to develop a method for original signal reconstruction taking into account the instrumental function for a specific spectral components and the spectrometer configuration. It allows to increase the accuracy of measured parameters of the investigated plasma source and to measure absolute values of the plasma x-ray radiation intensity. As the instrumental function can hardly be calculated analytically we used the ray tracing computer simulations. The general idea of this method is to trace a large number of rays emitted from the source while they are transmitted through the optical system. We studied the dependence of the result on both simulation parameters (the number of rays and their initial distribution) and the parameters of the system under study (geometry of elements, reflectivity and transparent function, etc). The simulations were performed using our own ray tracing code. Using this code we studied the dispersion for the spherical quartz crystal with the curvature of 150 mm. The influence of the following parameters is considered: the position of x-ray source, the size of the source, and the crystal surface reflectivity function. As the simulation result the dependence of the reflected spectral line intensity on the wavelength for different scattering angles was obtained. The areas on the crystal surface that meet the Bragg condition for different spectral components were determined and visualized depending on the reflectivity function. Moreover, we examined the influence of the reflectivity function on image aberration in monochromatic backlight of the object.

DESCRIPTION OF DIFFUSION IN U AND U–Mo FROM THE ATOMISTIC SIMULATIONS

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Diffusion processes play an important role in the behavior of materials under reactor irradiation, so uranium and its alloys are actively explored [1]. Measurement of self-diffusion coefficient show anomalously high diffusion mobility in gamma-U compared to other bcc metals. However, the mechanisms of diffusion is still not clear. This paper discusses the signs of interstitial and vacancy diffusion mechanism in the gamma-phase of uranium and uranium-molybdenum contact.

In this work basing on the molecular dynamics simulations we have evaluated the formation energy and volume of various defects in U and U-Mo alloy. The system is investigated at high temperatures, within which a gamma-U is stable. The calculations were performed using potentials presented in work [2]. Results showed that energy and volume of formation for interstices in the gamma-U are less than for vacancies. Hence, the concentration of interstitials dominates and should govern self-diffusion under compression.

In the second part of work the model of the interdiffusion at the contact of gamma-U and Mo is presented. These materials, presumably, have different diffusion mechanisms. It is interesting to find out which mechanism dominates in the interdiffusion. The model is based on the results of MD calculations of the diffusivities of the components as a function of their concentrations. It is specified by differential equations of diffusion for each material. With this system, the dependence of uranium (molybdenum) concentration is considered in time and coordinate space. MD model of uranium and molybdenum contact was also created and explored. It is going to be compared with results of previous calculations and experimental data.

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THE KINETICS OF POINT DEFECTS IN METALS UNDER ION IRRADIATION

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Radiations of different types during their interaction with metal violate its periodic structure, and cause an appearance of different types of defects that change mechanical properties of irradiated material. At high doses of irradiation, it can lead to swelling of structural materials.

Primary and secondary processes of the defects formation can be allocated. The primary processes are the development of a cascade of atomic collisions and the formation of point defects, and the secondary processes are migration and association of the resulting defects. Modeling an irradiation process of a copper plate for studying the formation and evolution of point defects, that is vacancies and interstitials, is presented in this work. The plate is considered to be infinitely long, so a one-axis task is solved. Homogeneous (no streams of defects in a sample) and inhomogeneous cases are studied. Irradiation is pulse-like. The Euler scheme is used to fulfill the homogeneous task, a central-difference scheme is used to solve the inhomogeneous task. Atomic concentrations of vacancies and interstitials in the plate of copper are obtained as a result of calculations.

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MOLYBDENUM ATOMS YIELD IN PULSE UV LASER PHOTOLYSIS OF $Mo(CO)_6$

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Laser photo-dissociation of metal carbonyls leads to supersaturated metal vapor formation [1].

As a result the metal nanoparticles growth can be observed. This study is devoted to time resolved measurements of Mo atoms concentration in the ground state producing by laser pulse photo-dissociation of $Mo(CO)_6$ in the mixture with bath gases at the room temperature. These data are important for the investigation of kinetics of small clusters and following nanoparticles growth. The experiments were performed in a quartz reaction cell 0.5 cm^3 in a volume, filled with vapor of $Mo(CO)_6$ in the mixture

with argon. This mixture was irradiated by one Nd:Yag laser pulse at a wavelength of 266 nm. The laser pulse duration was 12 ns and the laser energy density was in the range of 0.02–0.17 J/cm^2.

Atomic resonance absorption spectroscopy technique was used to measure concentration of molybdenum atoms formed in the photolysis of $Mo(CO)_6$. The yield of molybdenum atoms in the ground state occurs due to process of spontaneous quenching of excited states or in collisions with surrounding gas molecules. Excited Mo atoms are formed in dissociation of $Mo(CO)_6$ molecules owing to absorption of two or more photons at 266 nm. In the experiments the consumption of Mo atoms was also observed and was explained by the small Mo clusters formation and secondary reactions. The influence of various bath gases (Ar, He, CO_2, CH_4, N_2, CO) on Mo atoms yield was found to be negligible. From the other side, the bath gas influenced on the processes of Mo atoms consumption. The kinetic mechanism of Mo atoms clusterization is studied by kinetic modeling using basic reactions responsible for Mo atoms consumption. Obtained results can be used for development of kinetic models of the early stages of Mo nanoparticles growth.

This work has been supported by the Russian Foundation for Basic Research (grant No 14-08-00505).

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CO-PYROLYSIS AND CO-FIRING OF MIXTURES FROM LOW-GRADE COAL AND BIOMASS

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Interest to the co-firing of different kinds of coal and different types of biomass is caused by tendency to wider usage of renewable hydrocarbon raw materials in energy purpose and to enhance the consumer characteristics of low-grade fossil solid fuels. In this paper as initial raw materials there were considered coal slack, straw and their mixtures. Investigations were carried out with the help of the analyzer SDT Q600, which allowed applying the methods of thermogravimetric analysis (TGA) and differential scanning calorimetry DSC). The experiments were carried out in inert (nitrogen) and air atmosphere. The heating rate was equal to 20°C/min. Application of TGA and DSC to investigations of coal slack and straw

mixtures with different mass ratio between the mentioned raw materials allowed detecting the condition at which non-additivity of mixture properties as respects to the rate of thermal decomposition and heat generation during pyrolysis and burning takes place. Similar investigations were fulfilled for mixtures of coal slack and straw subjected to preliminary thermal treatment (torrefaction).

SIMULATION OF A PROCESS FOR THE TWO-STAGE THERMAL CONVERSION OF BIOMASS INTO THE SYNTHESIS GAS

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There is high interest to the problem of development of power generation systems on the renewable energy source – biomass. One way to solve this problem is thermal conversion of biomass, such as a two-stage thermal conversion method, that have been developed at the Joint Institute for High Temperatures RAS. The first stage is pyrolysis of biomass. On the second stage the pyrolysis products is blown through the porous biomass residue at the temperature of about 1000°C, where there are their conversion into hydrogen and carbon monoxide. The volume of syngas is about 1.4 Nm^3 per kg of processed biomass and its calorific value is about 11 MJ/Nm^3. The paper describes the process simulation results of synthesis gas obtaining from biomass. In accordance with the tests of the pilot plant of electric power up to 50 kW, based on the two-stage pyrolysis-cracking process, the power plant combined with gas-diesel engine has a relatively low coefficient of energy conversion efficiency of initial biomass into electric power. This is due to incomplete conversion of the biomass into synthesis gas. The potential of increasing of the pilot plant efficiency was analyzed. There are two major ways to improve the energy efficiency of the power plant: (1) complete gasification of biomass residue by means of water steam, (2) burning of biomass residue in the furnace for the own heat needs.

A model was developed describing energy and mass balance, that allowed to estimate the parameters of biomass processing unit for both cases. The implementation of any of the suggested ways will significantly rise (by about a third) the overall energy conversion efficiency of power plant.

THE PYROLYSIS PROCESS OF SEWAGE SLUDGE

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Problems of environmentally friendly biowaste recovery are acute for all developed country. In spite of the ecological requirements in development of recovery technologies, it is necessary to provide economical practicability of applied recovery methods. As such closed-loop technologies are the biggest interest what provide waste treatment facilities by energy for satisfaction of auxiliaries. The scheme of sewage sludge recovery to give gaseous energy fuel was developed. A available scheme includes a chemical dehydration and thermal drying processes, a pyrolysis of solid residue and a pyrolytic cracking of volatile pyrolysis products. The gaseous product of pyrolysis and cracking is syngas that can be used as fuel in device generated energy. The experimental researches of the sludge sample pyrolysis process were carried out. The chart of reaction gaseous-product composition from the process conditions and the reaction heats of thermal sludge solid-body decomposition at the different temperatures were investigated. The composition of pyrolysis gases, calorific capacitance of the sludge samples and pyrolysis gases, the reaction heats of sludge pyrolysis at the different temperatures of process were determined.

VIRTUAL WATER MOLECULE DISSOCIATION IN AN ALTERNATING ELECTRIC FIELDS

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Results are presented for the numerical simulation of the real water molecule dissociation based on its two-dimensional analogue, namely, the virtual molecule (VM) dissociation in an electromagnetic field with a different time dependence of the electric field amplitude. The proposed VM model provides the condition of coincidence between the fundamental eigenfrequencies of the real molecule and its analogue. The bond length and atomic mass are renormalized so that the VM molecule should steadily exist for a long time interval. Numerical simulation of the impact of electromagnetic fields on the VM allows us to consider the dynamics of the atoms until the bonds break. Various scenarios of the molecular system behavior and necessary conditions for the intramolecular energy redistri-

bution have been investigated. It is shown that in some cases breaking of one of the VM bonds inevitably leads to the VM dissociation as a whole. As a result of numerical simulation, it has been established that the bond breaking has a threshold character, i.e., dissociation is not observed at the external force, which is below a certain value. Computations are performed for the value of the electric field amplitude, the shape of the electric potential and its potential difference. Optimum parameters of VM dissociation have been determined.

The considered scientific problem in the present conditions of depletion of hydrocarbon resources is an actual challenge with both theoretical and practical point of view. The results shows key opportunity to implement the research solutions in the field of hydrogen energy.

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SHOCK RESPONSE OF MAGNESIUM SINGLE CRYSTALS AT NORMAL AND ELEVATED TEMPERATURES

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A series of magnesium single crystals, from 0.2 to 3 mm thick, were shock loaded in directions parallel and perpendicular to the c-axis of the hexagonal closed packed (hcp) structure and at 45° to the c-axis. Shock compression along the c-axis is associated with the largest Hugoniot elastic limit (HEL) for this material. Microscopic observation of recovered c-cut samples demonstrated intense twinning with a greater density of twins near the impact surface. The low-energy basal slip was activated by shock loading along the inclined direction and has the smallest HEL. In all cases, we observe the decay of the elastic precursor wave and growth of the HEL with increasing temperature. For the inclined shock compression after the HEL, two plastic waves were found where the stress level of the first plastic wave depends on the peak shock stress. Finally, the largest spall strength was along the transversal direction and the smallest in the off-axis direction. The fracture surface of the sample of transversal orientation contains numerous groves oriented along the base planes of the crystals.

HALIDE BASED SHOCK-WAVE TREATMENT OF FLUID-RICH NATURAL PHASES

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The high-pressure behavior of fluid bearing phases is currently an object of great interest. This includes the chemical and structural behavior

of water bearing silicates in the time of subduction and also the behavior of carbonates (deep carbon cycle, Deep Carbon Observatory [1]).

In the current time the research of the shock wave behavior of carbonates is limited to the degassing behavior at impact events like Chixculub [2]. In this case carbonates shows a decay into CaO and CO_2 at elevated temperatures and a fast recombination along the release path [3], resulting the recovering of calcite without any high pressure phases. This method is not sufficient for the investigation of the HP-behavior of CO_2 and H_2O-rich natural phases. For this reason a new method was developed, based on the Imdedance Corrected Container [4] without adiabatic decompression of the sample powder [5] under using of halides (in first steps NaCl). For first experiments the kaolinite KGa-28 from the American Clay Society as reference material was used. The experiments were performed at pressures from 15 and 20 GPa and at approximately 110 GPa. First results shows a complete melting and amorphisation of the kaolinite under using of copper powder, the 27Al-NMR shows only the common 4-,5- and sixfold Al-coordination, higher coordinated silicium was not observed. The amorphous Si-Al-composition covers partially the Cu-metal grains and there complete dissolution with HNO_3 was impossible. On the other hand the samples treated under using of NaCl shows a crystalline structure and different Al-coordination numbers, depending on pressure and relative temperature under using the NMR-spectroscopy. In the current time further measurements were performed.

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ELECTRICAL RESISTANCE OF SHOCKED VANADIUM IN THE RANGE OF ELASTIC PHASE TRANSITION

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A series of multiple shock experiments were performed on vanadium at shock pressure ranging from 10-40 GPa and 40-120 GPa. Electrical resistance profiles measured for thin foil were used to estimate the volume-temperature dependence of vanadium electrical resistance under high-pressure high-temperature range.

A phase transition at some shock pressure that may be the body-centered cubic (BCC) to rhombohedral structure was discussed by the deviation of the shock volume-temperature dependence of vanadium electrical resistance from Bloch-Gruneisen law against shock pressure. The transition pressure is consistent with the results from literature diamond anvil cell [1], and shock experiments [2].

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ELECTRICAL CONDUCTIVITY AND THERMOPHYSICAL PROPERTIES OF LITHIUM HYDRIDE AND LITHIUM DEUTERIDE IN THE MEGABAR SHOCK PRESSURE RANGE

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The region of a high electrical conductivity of lithium hydride is experimentally determined in the pressure range 100-150 GPa and the temperature range 2000-3000 K of multiple shock compression. This result is used

to construct thermodynamic potentials for the two polymorphic modifications of lithium hydride (B1, B2), and these potentials make it possible to calculate its thermophysical properties in the shock pressure range 80-1200 GPa. The calculated and experimental results are analyzed to determine the B1-B2 equilibrium line for the polymorphic modifications of lithium hydride at pressure up to 300 GPa and temperature range 2-3 KK [1]. This work was supported by ROSATOM contract H.4x.44.90.13.1112.

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HYDROSTATIC AND SHOCK-WAVE COMPRESSION OF A MOLECULAR CRYSTAL

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Thermodynamics of high-molecular organic compounds and especially metastable chemical compounds, both being energy-saturated materials, turns out to be a poorly studied area despite its practical importance. Theoretical determination of relationships characterizing behavior of solid energy-saturated materials runs into difficulties as they belong to molecular crystals and molecules constituting a crystal have great many internal degrees of freedom. The paper analyzes experimental data on the hydrostatic and shock-wave compression of the energy-saturated material. The Mie–Grüneisen–Debye semi-empirical equation of state based on the Helmholtz potential is used to describe thermodynamic properties of metastable molecular crystals without phase transitions taken into account. The equation of state describes experimental data on isothermal compression of a molecular crystal with the above data given by the powder diffraction analysis using diamond anvils. An expression for the Hugoniot curve satisfactorily describes the data on shock compression of the material having different initial porosity. The proposed equation of state is expected to give higher-accuracy description of thermodynamic properties of the energy-saturated material in numerical simulation of shock-wave and detonation processes.

ACTION OF SHOCK WAVE LOADING ON SELENIUM NANOCOMPOSITES

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Selenium nanocomposites have promising applications as materials for electronics, photonics and pharmacology. But the properties of elemental selenium in these materials are not investigated completely. Selenium has many amorphous and crystalline modifications. Amorphous forms can transfer in crystalline ones at heating or static pressure about 14GPa. But nanosized selenium differs from compact one and has a transfer at a more high pressure which depends on properties of nanoparticles- its sizes and surrounding matrixes. For understanding of fundamental properties of these composites shock wave action with high resolution and express X-ray study is the very significant method. Selenium nanocomposites were obtained after drying of water solutions of polyvinyl alcohol contained nanosized selenium. Last one was the result of reaction of reduction of ammonium selenite by hydrazine-hydrate. Samples of nanocomposites were investigated before and after shock wave action. Optical, electronic microscopy, conventional X-ray diffraction and the small angle X-ray scattering method with synchrotron radiation of collider VEPP-3 were used. Shock waves were results of explosion in special chamber. Experimental data are analyzed and discussed.

PULSE LOADING OF GLYCEROL BY ELECTRIC EXPLOSION OF WIRE

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Experimental investigation of dynamic (strain rate 10^5 - 10^7 s^{-1}) compression of glycerol (GOST 6824-96) was carried out. Shock wave loading produced by electrical wire explosion [1]. Free surface velocity profiles were obtained using VISAR velocitymeter. Free surface was measured on the thin membrane of metallized film. It was found that the profiles are self-similar and the dependence of the strain rate at the compression wave

front on the wave amplitude has the form of a power law relation with the exponent of 3.2 for water [1] and of about 4 for glycerol which is close to the values obtained for metals [3] [5]. This power law relation can be related to the non-newtonian behavior [4]. We have observed multiple (up to 15) reverberations in the spall plate. Also we have observed change of refraction index of glycerol in the area close to the exploded wire. We can conclude that in glycerol the spall plate exists for longer time and dissipation of the acoustic wave is low.We suppose that for the investigated range of strain rates the non-Newtonian behavior is related to the plastic flow mechanisms as observed in solids. This work was supported by the Russian Foundation for Basic Research, project nos. $14-01-96012r_ural_a$, $14-01-00842-A$.

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ANOMALOUS COMPRESSIBILITY AND SPALL STRENGTH OF CERIUM AND DOCOSANE UNDER SHOCK-WAVE ACTION

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In this work we determined the shear stress and evolution of compression wave in the area of cerium anomalous compressibility. The value of longitudinal stress at which the alpha-beta phase transition occurs is also determined. It is shown that the phase transition pressure, under dynamic and static compression coincide and is equal to 0.8 GPa. The dependence of spall strength of cerium on the strain rate is investigated. At its increase from 1.5×10^4 to 8.5×10^5 s^{-1} the spall strength rises from 0.3 to 0.8 GPa. Similar experiments with docosane in solid and liquid state have been onducted. It was shown that the solid docosane demonstrate an elastic-plastic properties and has abnormal compressibility at pressures

below 100 MPa. It was found that the strength of docosane remains practically constant and equals to about 24 MPa when passing through the melting point.

DEVELOPMENT OF TARGETS FOR SHOCK-WAVE EXPERIMENTS AT PRIOR—PROTON MICROSCOPE FOR FAIR

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Materials with anomalous compressibility under shock loading conditions (cerium, docosane, porous medium) can be used as targets for PRIOR—proton microscope for FAIR. They are very interesting subjects for proton radiography studies due to the anomalous structure of the resulting compression waves and the unusually high jumps of density observed during their phase transitions. Abnormal compressibility may occur due to thermodynamic properties (cerium) and/or irreversible deformation dynamics (the porous medium). Theoretical models for describing the anomalous compressibility and behavior of different materials under extreme conditions are still not developed.

Another type of materials which are interested as targets are heterogeneous media with a strong anisotropy of physical properties (e.g. carbon composites, fiberglass, organo-plastics). Shock wave compression of carbon plastics generates a two-wave configuration associated with different propagation velocities along the reinforcing fibers and the polymer matrix. The range of the existence of the two-wave configuration depending on the wave parameters and the stress amplitude should be determined. This is needed for the development of models which adequately describe the behavior of materials under conditions of extreme compression. For this one has to measure the density of the sample under shock loading conditions which can be uniquely done by proton radiography.

The third type of targets are connected with spall strength study of inert and chemically active liquids. This phenomenon is of great scientific interest because it allows to obtain negative pressures in liquids and to reach regions of the phase diagram which cannot be achieved by other methods. The kinetics of homogeneous nucleation leading to pore formation, the subsequent growth of which results in spalling, has not been studied in detail, although it is widely used to interpret the data on pulse destruction of liquids. The proton radiography method will allow to di-

rectly observe the dynamics of pore formation, which shows up as a change of the liquid density in the fracture zone.

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MANUFACTURING OF SILICON NITRIDE HIGH PRESSURE PHASE IN PLANE RECOVERY AMPOULES OF HIGHER CAPACITY

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Silicon nitride high pressure phase (γ-phase) is close in bond nature to cubic boron nitride and diamond and as well as these materials shows significant hardness. The research of transformation degree of silicon nitride to γ-phase in recovery ampoules depending on shock compression parameters is presented in [1–3]. The attempts to manufacture large portions of about several grams per one experiment are undertaken in [4, 5]. Last two approaches showed some disadvantages. In the present work we manufactured of several grams of γ-phase per one experiment in plane recovery ampoules of higher capacity using high temperature shock compression method (HTSC) [6]. Tablet samples of 1,5 mm thickness and 20, 60, and 100 mm diameter were prepared of mixture Si_3N_4/KBr-40/60 wt.%. The loading of the samples to approximately 50 GPa in recovery ampoules was carried out with Al and stainless steel flyers accelerated by explosive throwing devices. New approach in constructing of recovery ampoules (copper core — steel cover) allowed decreasing the losses of the material of samples significantly. The highest yield was achieved in experiments with Al flyers.

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EXPLOSIVE COMPACTION OF MIXTURE WC+Co ON AXIAL SYMMETRIC SCHEME

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In this work, the task to develop and optimize schemes of explosive compaction of powder mixtures of solid materials with a metal band was resolve. Experiments on explosive compaction of mixtures of tungsten carbide (WC) and cobalt (Co) in the cylindrical ampulas of conservation has been performed. A numerical simulation of the propagation of shock waves on a two-phase porous medium WC+Co was hold. On the basis of experimental and numerical studies of shock wave propagation the optimal conditions of explosive compaction of a two-phase porous medium are defined. It is shown that the most advantageous for obtaining a uniform mixture of solid compact powder WC+Co 9:1 by volume axially symmetric with the central mandrel circuit is compaction mode corresponding to the detonation velocity explosive charge 4,6 km/s, followed by sintering.

PULSE COMPRESSION OF THE Ni AND Al MICRON POWDERS MIXTURE IN CYLINDRICAL RECOVERY AMPOULES

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The assemblies with cylindrical recovery ampoules for dynamic compression of the Ni-Al powders mixture and initiating the chemical synthesis of NiAl intermetallic are tested. The chemical synthesis scheme based on the detonation of a RDX cylindrical charge, which is located along the axis of ampoule. The detonation wave sliding along the surface of the ampoule caused a compression wave [1]. The pressure profile on the ampoule surface depends on the design features of the explosive device. Charge of RDX had a diameter of 57 mm and a length of 70–100 mm and its weight varied from 160 to 300 g. The diameter of the cavities in ampoules equaled 5–8 mm. Analysis of the shock-wave dynamics in the construction of various explosive assemblies showed that the dynamic effect on the walls of ampoules continues for 30 ms or more, and ranges up to 25 GPa. Estimate of

the ampoule temperature immediately after loading, based on measuring the speed of decline after the experiment, gave values of 400–450 K.

Starting material was a powdered mixture 0.7Ni + 0.3Al and was pressed into the cavity to the density 0.55–0.70 g/cm^3. The porosity of the compacted mixture was 0.31–0.42. After the shock-wave loading the X-ray analysis of stored compacted samples was made and distribution of porosity along their length was found. X-ray analysis showed the presence of a number of NiAl intermetallic phases, porosity distribution along the length of the sample has an inverse correlation with pulse pressure on the surface of the ampoule and the time of its action: the lower the porosity is shown at large pressure.

The data obtained allow to estimate the density of the recovery samples (4.5–5.8 g/cm^3), and also the residual porosity in these ampules after compression and synthesis concerning porosity of initial mixture (0.07–0.39). The density of the NiAl intermetallic taken equal to 6 g/cm^3.

The results obtained in the experiments are planned to use in experiments with nanosized and microsized powders of the starting components for obtaining more dense NiAl samples.

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SUBMICROSECOND STRENGTH OF COMPOSITE MATERIAL OBTAINED BY SHOCK COMPRESSING OF THE POWDER MIXTURE Al/Al_2O_3

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Explosive compaction of systems based on metal powder is a promising direction in the development of the new structural materials. In this case, the study of composite based on powders over the wide range of stain rate 10^{-5} s^{-1} to 10^5 s^{-1} to identify the mechanisms of deformation and fracture and their connection with the internal microstructure is of interest. The processes of high strain rate and fracture caused by the shock wave in such materials have not been studied at all. In this work the samples were synthesized of powder composite material by the explosive compaction. The initial synthesis mixture consisted of powders ASD-6 (average size of 18 microns) and aluminum oxide (average size 36 nm). The mixture was premixed in a tumble mixer for 24 hour. The amount of Al_2O_3 in the mixture

was 10% by weight. The resulting mixture was placed in an axisymmetric container. The container was a copper tube with a diameter of 32 mm and a length of 350 mm (wall thickness 1 mm). Explosive compaction occurred under the action of the detonation products of industrial explosive Uglenit E-6 with a detonation velocity of 2300 ± 200 m/s. As a result the composite with density 2.65 g/cm^3 was obtained by synthesizing. The measured longitudinal sound velocity was 6.10 ± 0.1 km/s. Vickers microhardness was 106 ± 6 kg/mm^2. Using electron microscopy and X-ray diffraction data on the composite structure, the parameters of the crystal structure and phase composition were found. For the shock-wave experiments the samples of 2 mm and 5 mm were cut. The plane shock waves in the samples were generated by impacts of aluminium flyer plates of 0.85 mm and 2.0 mm in thickness with velocities of 630 ± 30 m/s. The free surface velocity histories were monitored with the VISAR. The measured values of the Hugoniot elastic limit in the composite sample with thicknesses of 2 mm and 5 mm were 0.24 ± 0.01 GPa and 0.2 ± 0.01 GPa. The dynamic strength of the composite was 0.4 ± 0.01 GPa and 0.35 ± 0.01 GPa for samples 2 mm and 5 mm in thickness.

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MOBILE LABORATORY "EXPLOSIVE DESTRUCTION OF NATURAL MATERIALS". PART 2: EXPERIMENTAL STUDY OF THE BEHAVIOR OF ICE AND LIMESTONE UNDER EXPLOSION LOADING

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Nowadays, theoretical and experimental study of the behavior of some natural materials (ice, granite, limestone, rocks), have not lost their relevance. This is due to the need to increase the extraction of natural resources in areas of permafrost and the Far North, the development of transport links in the Arctic and the development of new ways to fight ice jams. In the next few years, the Russian government plans to come to grips with the development of the Arctic zone. It is about recreating a new transport infrastructure, implementing large-scale programs of extraction

of natural resources, military build-up. Therefore, a need for new experimental data on shock-explosive loading of natural materials for testing techniques developed numerical simulation [1].

In this paper we study the behavior of natural materials with explosive shock loads. The fullscale experiments were conducted in cooperation with "KuzbasSpetsVzryv" in Tomsk region of the Siberian. As objects of study selected limestone and medium first-year ice. Figure illustrates the process of preparation for the experiments. The purpose of this work was to identify the main mechanism and regularities of their explosive loading. In studying the behavior of limestone under explosive loads varied mass of explosives from 5 to 50 kg. The diameter and depth of the wells remained constant at 11 and 560 cm, respectively. Some wells contained water, which reached the level of 200 cm or more. The air temperature was equal to 3°C. In the experiment recorded only the diameter of the crater, which reached 120 cm. In studying the behavior of ice during blasting loads varied mass of explosives. The explosive weight was equal to 4 and 8 kg. The freshwater ice thickness was 70 cm. The depth of water under the ice cover was about 7 meters. The flow of water was low. The water temperature was equal 4°C. After the explosion in the ice formed on the lane in diameter from 2 to 4.3 meters.

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SUPERCONDUCTIVITY OF Al/Al_2O_3 INTERFACE FORMED BY SHOCK-WAVE PRESSURE

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This work is further work [1]. A mixture of Al and Al_2O_3 has been subjected to a shock-wave pressure of ≈170 kbar, followed by vacuum-encapsulating and quenching of the product to liquid nitrogen. The ac magnetic susceptibility measurements of the samples have revealed metastable superconductivity with $T_c \approx 37$ K, characterized by glassy dynamics of the shielding currents below T_c. Comparison of the ac sus-

ceptibility and the dc magnetization measurements infers that the superconductivity arises within the interfacial granular layer formed between metallic Al and its oxide due to the shock-wave treatment. This work was supported by RFBR grant No. 13-02-01217.

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SHOCK WAVE VELOCITY MEASURING SYSTEM BASED ON VERNIER VISAR-TYPE INTERFEROMETERS

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The uniqueness of shock wave physics experiments and inability to repeat them under identical conditions place heavy demands on output data. Most informative contactless method in such experiments is Doppler interferometry, that allows to carry out continuous surface velocity measurements. Today quadrature-differential VISAR systems are the most widespread laser systems for velocity measurements. They have earned a reputation as reliable, convenient and relatively inexpensive devices providing sufficient accuracy and time resolution for most measurements. However, these measuring systems have a number of limitations due to properties of optical layout. In particular, the standard quadrature-differential interferometers are designed for the simultaneous measurement of the velocity of only one point on an object (or more precisely, they measure average speed of $\sim 10^{-5}$ cm^2 area). Moreover, significant problem is "missing" of interference periods that can occur in the signal if photographic system's time resolution is not enough. This "missing" is usually observed at the shock front (with times < 10 ns) and can lead to significant errors in the recorded velocity absolute value.

This paper presents a laser system for measuring the surface velocity in shock wave experiments. This system is combination of optical units producing signal frequency analysis and electronic components producing photoelectric conversion interconnected by optical fibers. Two optical units form vernier system with polarization coding of quadrature-differential signals. Using delay etalons with different optical length allows to extend system's dynamic range and obtain exact parameters of fast shock front even

with interference periods "missing". Interferometers optical layout allows each one to produce independent analysis of up to 7 optical channels.

The basic operations with the interferometer may be performed remotely from a PC using special software and a remote control unit. Built-in Ethernet interface allows to adjust interferometers remotely, control elements status and perform remote recording of digital signals. Using fast photomultipliers (Hamamatsu R9880) as photodetectors allowed to reach the operating speed of 0.8 ns, with the possibility of using laser with power < 1W as a probe source when working with low reflection surfaces, including diffuse ones.

TUBULAR EXPLOSIVE DEVICES FOR QUASI-ISENTROPIC COMPRESSION OF GASES TO PRESSURES OF 200–400 GPa

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Tubular explosive devices with the speed of waves in the magnesium rod 15 km/s for multiple and isentropic compression of gases up to 200–400 GPa have been created. A series of cells for measuring the conductive properties of sapphire and gases are designed and manufactured. The size of region for one-dimensional and uniform compression of helium inside of the experimental cell have been determined by two-dimensional numerical hydrodynamic modeling. It is established that for a cell with an initial thickness of 2 mm with helium at a temperature of 78 K and the initial pressure 20 MPa required conditions of homogeneity and one-dimensionality of the gas compression is performed in the central region of the cell with diameter 6 mm.

To increase the size of area of homogeneous and one-dimensional compression it is proposed to increase the diameter of the tube copper liner 1.5 times with a corresponding increase in the mass of charge up to 13.5 kg.

STUDY OF DEFECT INDUCED METASTABLE STATES, PLASTICITY AND DAMAGE MECHANISMS IN SHOCKED MATERIALS

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Experimental and theoretical study is devoted to the links of defect induced metastable states, elasto-plastic and damage-failure transitions in shocked materials as specific type of criticality (structural-scaling transitions) in out-of equilibrium system "solid with mesodefects". It was shown that kinetics of structural-scaling transition is related to the dynamics of two internal variables: defect density tensor (geometrical part of defect induced strain) and structural-scaling parameter characterizing the current sensitivity of material to defect growth and representing the ratio of mean sizes of defects and spacing between defects. Two critical values of structural-scaling parameter, that were established by statistical thermodynamics of solid with defects, determine characteristic types of defect induced metastability that provides qualitative changes in multiscale defects dynamics due to the subjection of solid responses to specific types of collective modes of defects (autosolitary modes that are characteristic for plasticity and transforming into blow-up damage localization modes). These modes have the nature of self-similar solutions for defect evolution equations in terms of mentioned variables [1]. Excitation of these modes due to the metastability decomposition were used for the interpretation of original "in-situ" experiments: elasto-plastic transition in shocked metals (elastic precursor decay [2], the four power law universality [3]); "resonance" excitation of damage localization ("dynamic branch" of numerous spall failure in quartz and ceramic rods, "delayed failure" in compressed fused quartz rods [4]), power spatial-temporal universality of fragmentation statistics in quartz and ceramics based on the "in-situ" fractoluminescence data [5].

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HOMOGENEOUS NUCLEATION OF DISLOCATIONS IN METALS UNDER UNIAXIAL DEFORMATION AND PURE SHEAR

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Dislocations are linear defects in the crystal lattice, their movement is a major mechanism of plastic deformation. Usually dislocations already exist in material. Homogeneous nucleation can be observed under dynamic loading, when the strain rate is so high that shear stresses do not have time to relax at the expense of reproduction and movement of existing dislocations [1]. Homogeneous nucleation of dislocations restricts the shear strength of perfect crystals. The report presents the results of molecular dynamics study of ideal shear strength of single crystals of aluminum, titanium, iron and nickel in a pure shear strain, uniaxial tension and compression. The simulation was performed using the package LAMMPS [2]. We consider a system consisting of different number of atoms at different temperatures and strain rates. Were defined shear stress at which the system begins to form dislocations and plastic deformation began. As can be seen from the simulation results, depending on the type of crystal lattice of metal better resists deformation of a certain type.

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ENERGY APPROACH TO KINETICS EQUATIONS FOR DISLOCATIONS AND TWINS AND ITS APPLICATION FOR HIGH STRAIN RATE COLLISION PROBLEMS

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Many investigations demonstrate that the energy release rate is almost constant both for plasticity and brittle fracture processes [1, 2]. In the case of plasticity, this feature allows one to propose a physically reasonable equations for kinetics of the defects [3–6]. In the case of mechanical twinning, it also enables one to formulate a new structural model as an extension of the dislocation model with only one additional parameter, characterizing the twin ability-the stacking fault energy of the material [5, 6]. Application of these model to numerical simulation of the high strain rate collision experiments, such as the flat plate collision or Taylor anvil on rod compaction test demonstrates a good fit with the available in literature experimental data [5]. Further applications of these models allow us to find the defect distribution in metal targets in a wide range of initial conditions and describe the contribution of dislocations and twins in the process of formation of the rod shape after the compaction for copper, aluminum and steel samples.

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DISLOCATION DENSITY AND CRYSTALLITE SIZE OF SHOCK WAVE LOADED TUNGSTEN AND SOME OTHER REFRACTORY COMPOUNDS FROM POWDER X-RAY

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Initial goal of the work was investigation of possibility nanomaterials preparation using shock waves. Variation of substructure parameters such as microstrain and crystallite size of some refractory materials after shock waves loadings has been investigated by powder XRD for this purpose. The shock wave compression was performed in planar recovery ampoules. The pressure (22–50 GPa) was generated by aluminum plates accelerated with explosive detonation products. Pure substances as well as their mixtures with potassium bromide were subjected to shock compression. Compression of the mixtures performed for lowering a post shock temperature and consequently decreasing annealing and recrystallization effects. Tungsten, silicon nitride, titanium nitride, tungsten carbide, zirconium diboride and dioxide were investigated. Silicon nitride, tungsten carbide and zirconium dioxide in contrast to titanium nitride and zirconium diboride possess polymorphism. This gains a better insight on nature of crystallite size variations under shock wave loading. Crystallite size reduction to nano level (< 100 nm) were not observed if no polymorphic transition occur under shock wave loading. Else if substances (silicon nitride, zirconium dioxide) undergo shock wave phase transformation then new nanocrystallite phase with crystallite size of 10–20 nm were formed. When phase transformation under shock wave loading does not occur, the reason of powder X-ray diffraction broadening is the considerable microstrains which most probably caused by rise of dislocation density.

This work was supported by the Presidium of the Russian Academy of Sciences fundamental research program “Matter under High Energy Density”.

SHOCK PRODUCED EJECTA FROM METALS: COMPARATIVE STUDY BY MOLECULAR DYNAMICS AND SMOOTHED PARTICLE HYDRODYNAMICS METHODS

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The machining of materials produces the regular micrometer-sized surface perturbations. As a shock arrives to the surface, the microscopic cumulative jets can be generated. The experimental investigation [1] of such ejecta of surface material demonstrates that characteristics of jets are directly connected with the material properties, the size of perturbation and the shock pressure. Results of recent simulations [2, 3] demonstrate that evolution of a micro-jet, from jet formation to its fragmentation, is not well understood. Experimental methods of observation of early stage of ejecta formation are still limited in terms of following a complete sequence of processes having microscale dimensions and nanoscale times. Therefore, simulations by the smoothed particle hydrodynamic (SPH) and molecular dynamic (MD) methods can shed of light on details of micro-jet evolution. SPH method is applicable in the wide range of amplitudes of perturbations, but it has problems in deciding on a fracture model and lack of surface tension of molten metal. In contrast to SPH approach, properties of material of interest in MD approach are defined with a potential of inter-atomic interaction. Thus, MD has no problems typical of SPH, but the size of simulated sample is too restricted in MD. In this study we demonstrate that the results of MD simulations with large enough number of atoms can be scaled well to the sizes of realistic samples. To validate such scaling the comparative MD and SPH simulations of tin and copper samples are performed. SPH simulation takes the realistic experimental sizes, while MD uses the proportionally scaled sizes of samples. It is shown that the velocity and mass distributions along the jets simulated by MD and SPH are in a good agreement. The observed difference in velocity of spikes between MD and experiments can be partially explained by a profound effect of surface tension on jets ejected from the small-scale samples.

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A MECHANISM OF WAVE FORMATION IN EXPLOSIVE WELDING. NUMERICAL SIMULATION

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The explosive welding of metals was discovered in experiments on cumulation in 1944–1946's. by a group of Soviet scientists under the guidance of M.A. Lavrentyev. Over the past years, the study of this phenomenon was the subject of many experimental works and theoretical models. The lack of adequate model about the nature of the waves on the boundary of metals naturally hinders the development of explosion welding technology because of parameters of welding seam (amplitude and wave lengths) are practically unpredictable.

In this work the mechanism of wave formation in explosive welding is discussed. The results of the direct numerical simulation of high-speed oblique collision of explosively accelerated plates are presented. The elastic-plastic model of media motion [1], wide-range equations of state for metals [2], the equation of state of explosives, explosion products and kinetics of decomposition of explosive substances [3] were used in two-dimensional numerical simulations.

The mechanisms of the initial instability and the wave formation were observed. It is shown that that the wave formation is described by Kudinov-Koroteev mechanism [4]. The wave lengths obtained in numerical simulation is closed to the experimental data.

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NUMERICAL SIMULATION OF EXPERIMENTS ON THE HIGH-SPEED COLLISION OF METAL PLATES

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The paper deals with modelling the high-speed collision of metal plates. In one-dimensional formulation equations of continuum mechanics are solved numerically, supplemented by equations of a model of dislocation plasticity [1–3], twinning [4] and destruction [2, 5]. For a numerical solution of equations we use a numerical method [3]. The thermodynamic state of matter is described by means of interpolation equations of state [6]. A comparison with experimental data [7] in the form of velocity profiles of the free rear surface of a target is presented. The influence of parameters of the models of plastic deformation [1–4] and destruction [2, 5] on the shape and height of an elastic precursor, the shape and amplitude of the plastic shock and rarefaction waves as well as the position of a spall pulse are analyzed. The calculations were performed for aluminum, copper and iron.

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NON-ISENTROPIC LAYERS IN CONDENSED MATTER AT SHOCK AND RAMP LOADING

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In the framework of the ideal fluid dynamics approach, the temperature and entropy values of a medium undergo a jump increase in the shock front as well as on contact interface between different materials after the shock wave propagation, but remain constant behind the shock front out of the contact interface. In real condensed matter, the shock fronts and transition regions near the interfaces have finite thicknesses; therefore, the temperature field is disturbed around the interfaces. In the present work, such disturbances are numerically analyzed for the problems of formation of the steady shock wave at impact and ramp loading of metals, exit of the steady shock wave to the free surface, and the shock wave passing through the interface between two different materials. Theoretical analysis and computations show that the non-isentropic layers (the high-entropy ones with the temperature increase and the low-entropy ones with the temperature decrease) arise near the interfaces in the above problems of shock and ramp loading. The impact produces the high-entropy layer, while the ramp loading can result in the both high- and low-entropy layers. At the shock wave passing through the interface, the high-entropy layer is formed in the lower-impedance material and the low-entropy—in the higher-impedance one. These high- and low-entropy layers should be taken into account in simulations of shock-wave processes in thin targets or in other cases where surface effects are important. For example, melting can take place in the high-entropy layer on the interface between colliding plates at shock intensities lower than the bulk-melting threshold; also, the temperature perturbations near the studied surface can affect the result of pyrometric measurements.

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NUMERICAL INVESTIGATION OF THE SHOCK WAVE PROPAGATION IN POLYMETHYLMETHACRYLATE

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Using Maxwell model of the viscoelastic medium [1], we study numerically the influence of the viscoelastic properties of polymethylmethacrylate on the change of the shock wave amplitude with the depth of propagating into the material sample. Parameters of the Maxwell model are chosen by comparison with the experimental data [2–4] on the high-speed impact of plates in order to fit the modeling results with the experimentally measured profiles of the free-surface velocity. A caloric equation of state is used to calculate the pressure upon the density and internal energy [5, 6]. It is shown that in a limit of weak shock waves, the accounting of the viscoelastic properties allows one to achieve a better coincidence of the calculated and experimental data on the magnitude of the shock wave velocity in comparison with the case of hydrodynamic calculations. In viscoelastic and hydrodynamic approaches, we have investigated the dynamics of the shock waves in polymethylmethacrylate initiated by pulses of pressure on the sample surface with durations of micro-, nano- and picosecond ranges. The calculation results show that the changes of the shock wave amplitude with the depth are approximately identical in the hydrodynamic and viscoelastic cases.

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PROPAGATION OF SHOCK WAVES AND FRACTURE IN THE COMPOSITE: NUMERICAL SIMULATION

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Calculation method for description of dynamics of the multiphase heterogeneous medium is presented. It is based on the two-level approach and takes into account finite rates of the stress relaxation between phases, the heat exchange, relative motion of phases and the friction between them. Conservation laws are formulated on the macroscopic level, while the laws of interaction between phases are obtained from the mesoscopic consideration, on the level of individual inclusions.

The method is applied to the problem of the high-current electron beam interaction with a material composed of aluminum matrix and copper inclusions. Plasticity and fracture models [1], [2] are used as a part of constitutive model for both component of the composite. Presence of inclusions considerably influence on the generation and propagation of stress waves. Destruction of the composite at the action of tensile stresses (back-side spallation) occurs through generation and growth of micro-voids in the phase with the smallest tensile strength.

Incorporation of copper inclusions in aluminum matrix leads to increase of the stress wave amplitude because of narrowing of the energy release zone and rise of the energy concentration. As the spall strength is determined by the weaker phase (aluminum), it leads to increase on 2-3 cm of the threshold target thickness, at with the back side spallation still takes place, in comparison with pure metal. At the irradiation intensities resulting in ablation, a considerable relative motion of matrix and inclusions takes place in the area of ablated material. In the ablated layer, the material with higher density falls behind the material with lower density.

In this work, the modeling of fracture is supported by the grant from the Russian Science Foundation (project 14-11-00538); the modeling of the shock wave propagation in composite is supported by the Ministry of Education and Science of Russia (competitive part of State Task of NIR CSU 3.1334.2014/K).

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DESTRUCTION OF CONCRETE BEAMS WITH METAL AND COMPOSITE REINFORCEMENT WITH IMPULSE ACTION

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The paper conducted a comprehensive experimental and theoretical study of the destruction of concrete beams, reinforced with steel and composite reinforcement. As composite reinforcement used carbon fiber and fiberglass. The aim of experimental investigations of wide laminated beams is the experimental determination of the characteristics of their deformation, fracture identification schemes and destruction of the elements of the layered structure in a short-term dynamic loading. Experimental beams consist of three different layers of reinforced thickness: fiber concrete, concrete, fiber concrete. Numerical simulation of the experimental conditions was carried out in full three-dimensional formulation within the phenomenological approach of continuum mechanics with explicit reinforcement. The behavior of steel reinforcement described elastoplastic model. In describing the behavior of composite reinforcement into account the anisotropy of the elastic and strength properties. Behavior of fiber-reinforced concrete and describe the elastic-fragile environment, taking into account the different strength under compression and tension. Used in the calculations author software package and an algorithm that allows to carry out parallel computing with high performance. Conclusions: - new experimental data on the fracture behavior of beams, changes in relative deformations of reinforcement, concrete and fiber-reinforced concrete, as well as the value of the dynamic load and support reactions over time; - the proposed model the behavior of fiber-reinforced concrete and adequately describes the dynamics of the stress and strain state of the process of destruction. - implemented the algorithm and the method of calculation allow us to study the behavior of the structure as a whole in the full three-dimensional dynamic formulation. - obtained numerical results are in good agreement with the experimental data; - regularities of damage depending on the scheme of reinforcement.

NUMERICAL SIMULATION OF DEFORMATION AND FRACTURE OF SPACE PROTECTIVE SHELL STRUCTURES FROM CONCRETE AND FIBER CONCRETE UNDER SHOCK-WAVE LOADING

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Shell structures are widely used in various fields ranging from oil and gas pipelines, various containers for storage and transport of materials, various types of aircraft: aircraft, ballistic missiles, to special constructions, designed to protect objects from natural and anthropogenic effects. When developing new constructions, besides the analysis of behavior of individual elements in different types of exposure necessary as well in the analysis of the behavior of the structure as a whole. Conducting this purpose field experiments involve, as a rule, with high material costs, and the experiment is not always give the full picture, especially for dynamic processes when necessary information about the parameters of interest at different times. Therefore, a need exists in the models and methods for the analysis and predict the behavior of structures under various types of operating loads and possible emergency situations. To adequately describe the behavior of structures must take into account the spatial nature realized in their stress-strain state (SSS), due to several factors: - The presence of elements that lead to geometric asymmetry; - The actual conditions of loading - usually they are not symmetrical; - Anisotropy of physical and mechanical properties of the materials of construction elements. The presence of at least one of these factors makes it necessary to analyze a three-dimensional setting, which is a very complex and time-consuming task, as in this case, in addition to creating an adequate model of the behavior of materials necessary to most effectively take account of the geometry and spatial arrangement of the various elements of the structure. The paper presents a model, method of calculation and the results of numerical simulation of the interaction of Boeing 747-400 aircraft with a protective sheath nuclear plant. The shell has a complex multi-layered honeycomb structure composed of layers of concrete and fiber concrete, fastened with steel trusses. Numerical simulation was carried out in a three-dimensional dynamic formulation, using the author's algorithm and software package, which implements an algorithm for constructing a grid of complex geometric objects.The dynamics of the stress-strain state and structural failure. On the basis of the developed method can be carried

out widely parametric numerical experiments on the selection of optimal design solutions.

NUMERICAL IMPLEMENTATION OF THE INCUBATION TIME FRACTURE CRITERION

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The paper is discussing problems connected with embedment of the incubation time criterion for brittle fracture into finite element computational schemes. Incubation time fracture criterion is reviewed, practical questions of its numerical implementation are extensively discussed. Several examples of how the incubation time fracture criterion can be used as fracture condition in finite element computations are given. The examples include simulations of dynamic crack propagation and arrest, impact crater formation (i.e. fracture in initially intact media), spall fracture in plates, propagation of cracks in pipelines. Applicability of the approach to model initiation, development and arrest of dynamic fracture is claimed.

NUMERICAL SIMULATION OF $ZrO_2(Y_2O_3)$ CERAMIC PLATE PENETRATION BY CYLINDRICAL PLUNGER

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In this paper dynamic fracture process due to high-speed impact of steel plunger into ceramic sample is simulated. The developed numerical model is based on finite element method and a concept of incubation time criterion, which is proven to be applicable in order to predict brittle fracture under high-rate deformation. Simulations were performed for $ZrO_2(Y_2O_3)$ ceramic plates. To characterize fracture process quantitatively fracture surface area parameter is introduced and controlled. This parameter gives the area of new surface created during dynamic fracture of a sample and is essentially connected to energetic peculiarities of fracture process. Multiple simulations with various parameters made it possible to explore dependencies of fracture area on plunger velocity and material properties. Energy required to create unit of fracture area at fracture initiation (dynamic analogue of Griffith surface energy) was evaluated and

was found to be an order of magnitude higher as comparing to its static value.

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NUMERICAL SOLUTION FOR PROBLEM OF IMPACT OF HETEROGENEOUS SOLIDS

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Numerical modeling of shock interaction of heterogeneous solids has a set of well-known difficulties. The strong deformation of a settlement grid localized in a zone of bodies contact limits possibilities of Lagrange approach. Washing out of contact boundaries is characteristic for an Euler method of the description. Existence of a large number of the contact boundaries taking place in heterogeneous material doesn't allow to use many from contact algorithms [1]. In particular possibility of the through calculation is required in this case.

In the present work two various variants of a particles method are used for calculation of impact of heterogeneous solids. The first method is a method of finite-size particles in cells (PIC-method) [2]. The second method is SPH-method [3] in which settlement cells are absent.

The wide range equations of a state (EOS) are necessary part of modern numerical hydrodynamics codes intended for calculation of high-speed impact [4]. Calculation of low-speed solids interaction demands use of the defining equations (DEQ) for the description of elastic-plastic behavior of material and spall destruction. However employments of EOS and DEQ lead to a set of features having in widely used and known numerical codes. Some of these features and ways of their account are considered in work.

Creation of the DE is required for heterogeneous materials when EOS of its components are known. The method of an elementary cell is widely used for calculation of defining equations [5].

Comparison of numerical results of impact of heterogeneous solids that receive by means of various particles methods are given. Conclusions are formulated about area of applicability of these methods.

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SELF-SIMILAR ASYMPTOTICS DESCRIBING NONLINEAR WAVES IN ELASTIC MEDIA WITH DISPERSION AND DISSIPATION

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Solutions of problems for the system of equations describing weakly nonlinear quasi-transverse waves in an elastic weakly anisotropic medium are studied analytically and numerically. It is assumed that dissipation and dispersion are important for small-scale processes. Dispersion is taken into account by terms involving the third derivatives of the shear strains with respect to the coordinate, in contrast to the previously considered case when dispersion was determined by terms with second derivatives. In large-scale processes, dispersion and dissipation can be neglected and the system of equations is hyperbolic. The indicated small-scale processes determine the structure of discontinuities and a set of admissible discontinuities (with a steady-state structure). This set is such that the solution of a self-similar Riemann problem constructed using solutions of hyperbolic equations and admissible discontinuities is not unique. Asymptotics of non-self-similar problems for equations with dissipation and dispersion were numerically found, and it appeared that they correspond to self-similar solutions of the Riemann problem. In the case of nonunique self-similar solutions, it is shown that the initial conditions specified as a smoothed step lead to a certain self-similar solution implemented as the asymptotics of the unsteady problem depending on the smoothing method.

VOLTAIC EFFECT IN BURNING HIGH-CALORIC (Zr+CuO+LiF)/(Zr+$BaCrO_4$+LiF) SANDWICH STRUCTURES

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Combustion of high-caloric (Zr+CuO+LiF)/(Zr+$BaCrO_4$+LiF) sandwich structures was found to be accompanied by generation of electric pulse with a halfwidth of around 1.0 s and 1.2–1.5 V in amplitude. Optical emission from the reaction zone was characterized by atomic emission spectra within the range 300–700 nm. Green mixtures and combustion products were explored by XRD and SEM. Combustion experiments were carried out by using a home-made experimental facility. For (Zr+CuO+LiF), (Zr+$BaCrO_4$+LiF), and (Zr+CuO+LiF)/(Zr+$BaCrO_4$+LiF) systems, the velocity of wave propagation was measured.

The results suggest that, in the system under consideration, the melted combustion products act as an source of electromotive force with a relatively low internal resistance while during cooling down (crystallization), as a source of current.

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IGNITION OF PYROPHORIC POWDERS: AN ENTRY-LEVEL MODEL

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Chemically prepared metal nanopowders are normally pyrophoric, i.e. liable to ignite spontaneously on exposure to air because of high reactivity and developed specific surface. In order to prevent accidents during their further processing, such powders are passivated (covered with a thin oxide film) in processes that last for dozen hours, which seriously restricts the mass production of nanopowders. On the other side, reliable theoretical models for spontaneous self-ignition of finely dispersed powders at room temperature have not been suggested so far. A deeper insight into the mechanism of the phenomenon would shed new light on the critical conditions for self-inflammation and thus would provide some clues for

optimization of the passivation process. The available models of ignition based on account of the retarding action of diffusion barriers seem inapplicable since, in terms of the above models, room-temperature inflammation is impossible at all because of low diffusivity of the oxide barrier.

In this work, we formulated and analyzed an entry-level model for ignition of pyrophoric powders. A planar infinitely long layer of porous condensed matter is in contact with gaseous oxidant at ambient temperature T0. The reaction of a porous solid with gas reactant is infiltration-controlled and yields a condensed combustion product. It is assumed that the temperatures of solid and gas in pores are the same (single-temperature model). Heat withdrawal from the reaction zone is assumed to proceed over the solid skeleton, and heat sink into the environment is neglected. Analysis of such a model in terms of the ignition theory gave the following results.

Depending on the width of the reaction zone, the ignition may get started in either one or two stages. The duration of each stage was evaluated by using approximate methods of combustion theory. In order to find out critical conditions for spontaneous inflammation, our model must be supplemented by either (i) the kinetic equations of combustion or (ii) the condition for formation of protective layer on the particles of solid reagent. Derived were parametric limits for the applicability of the model, and the influence of sample length on the ignition process was also explored.

NEW POSSIBILITIES TO STUDY DETONATION PHENOMENA AT THE VEPP-4M STORAGE RING FACILITIY

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A new station SEEMA-4 (Station for Experiments with Energetic Materials) was commissioned in 2014 on the collider VEPP-4 in Novosibirsk to study explosion and shock-wave processes.

At present, the SEEMA - 4 consists of a controllable SR gate at the entrance of the VEPP-4M beamline # 8; a monochromator with adjustable bandwidth; an SR beamline with diameter of 100 mm and length of 60 m; a unit for SR beam forming; an explosion chamber with movable beryllium

windows; a unit of detectors, which houses a DIMEX-3 detector and a prototype of silicon X-ray detector (with spatial resolution of 50 microns); a lead emergency trap for all types of radiation.

VEPP-4 collider enables generation of SR pulses (exposure time below 1 ns and an interval between pulses ranging from 150 ns to 1200 ns with uniform ring occupacy. The pulse trains with intervals downto 5 ns is also possible) to the SR beamline # 8.

The following dynamic experiments can be carried out at the new station:

1. measurement of density distribution in the fronts of shock and detonation waves;
2. measurement of dynamical distribution of bulk density, pressure and velocity field in spread of explosion products;
3. measurement of shock adiabats of continuous media;
4. measurement of dynamical distribution of small-angle X-ray scattering (SAXS) in shock-wave and detonation processes.

DETONATION OF MEHANOACTIVATED COMPOSITES OF ALUMINIUM AND AMMONIUM PERCHLORATE

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The main goal of this work is to develop scientific bases of production of new energetic materials with increased rates of energy release at the processes of combustion and detonation. Both grinding of the initial components with partial components diffusion and producing of the defects in crystal structure take place at mixture treating.

Mixing and activation of the components was carried out in the planetary mill Activator 2SL with steel balls and drums with water cooling. In the course of this study, the optimum conditions of mechanical activation of mixtures of ammonium perchlorate (AP) and Al were found so that the maximum uniform mixing of the components was provided in the absence of the reaction between the reagents under the selected processing conditions, which was shown by X-ray diffraction analysis and electron microscopy. For loose-packed mixes (20% of TMD), both the burning rates and D-values were measured in stainless steel tubes 10 mm in diameter. For Al/AP (20/80) the DDT length ranges from 65 to 75 mm and D ranges from 2.0 to 2.5 km/s.

The dependence of $D(\rho)$ was obtained for pressed charge with diameters (d) varied from 15 to 50 mm. The results of $D(\rho)$ have shown that in comparison with usual Al/AP mixes it is possible to receive essentially higher D-values that can be explained by increase in reactionary ability of the activated mixtures. For example for activated Al/AP charges with $d \geq 25$ mm D-values exceed approximately on 1 km/s the values predicted by D. Price dependence for nonactivated Al/AP [1].

The results of the present study allow us to consider mechanoactivation as a way to control the burning rate and detonation velocity. The short DDT-lengths and high sensitivity make it possible to consider MAECs Al + perchlorates as promising energetic materials for new initiating and incendiary compositions with increased requirements in the rates of energy release.

This work was supported by RFBR (grant No 12-03-00651) and the program of the Presidium of RAS The matter at the high density of energy.

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STABILIZATION OF UNSTABLE DETONATION WAVES IN NITROMETHANE MIXTURES WITH INERT DILUENTS

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Small additions of amines can influence the detonation properties of nitromethane (NM) and mixtures with diluents. This is especially shown in the change of critical values. It is expected that amines would influence the stability of detonation waves in the NM/acetone and NM/methanol solutions too. To investigate this phenomenon the laser interferometer VISAR was used for the recording of particle velocity profiles in detonation waves. The choice of the specific solution is determined by several conditions: the detonation front must be unstable, the size of heterogeneities must be an order of 10-50 microns so that they are visible when foil of the minimum thickness is used, and the concentration of the inert diluent must be far from the critical one. The NM/diluent solution with mass concentration of diluent from 10 to 20% satisfied all of these conditions. For NM/acetone (90/10) solution the disturbances of the detonation front do not attenuate at the detonation wave propagation through 7 microns Al

foil. It indicates that the size of the heterogeneities amplitude is comparable with the foil thickness, i.e. in the order of 10 microns. At the addition of 1% DETA the velocity profile is smooth, i.e. the detonation front becomes stabilized. Therefore, the addition of 1% DETA to the NM/acetone (90/10) solution results in the rejection of the instability of detonation front. In NM/acetone (80/20) solution the size of the instabilities was approximately 50 microns. The attempt to stabilize the detonation front by DETA additions resulted in a decrease of the heterogeneities size, but not a total absence, at 10% DETA their amplitude was about 10 microns. As in the case with acetone the addition of 1% DETA to the NM/methanol (90/10) solution results in the rejection of the instability of detonation front. But the attempt of stabilization of the detonation front by DETA additions for NM/methanol (80/20) solution resulted in a decrease of the heterogeneities size from 50 microns up to 10 microns at addition of 10% DETA. Thus, in the work it was shown that small additions of DETA not only influenced the critical parameters of detonation but resulted in the rejection of the instability of the detonation front in the NM/diluent solution with the size of the heterogeneities amplitude in the order of 10 microns.

AN APPROXIMATE METHOD FOR SOLVING THE PROBLEM OF THE ESTABLISHMENT OF CHEMICAL EQUILIBRIUM

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We developed the approximate method to calculate composition and thermodynamic parameters of detonation products based on the assumption of the existence of a partial chemical equilibrium. Without significant loss in accuracy, the respective stiff system of detailed kinetics differential equations can be replaced by a single differential equation and a system of algebraic equations. This method is always consistent with the detailed kinetic mechanism and can be used separately or in conjunction with the stiff system, replacing it when the bimolecular reactions reach the quasi-equilibrium state. The constituent equations of the model were derived and the respective computer code written. The applicability of the model was demonstrated by solving a model problem. It was shown that the proposed model can be used to calculate the characteristics of the detonation products flow-field after the induction period.

According [1] what we offer is not an approximate kinetic equation (as in [2]), but an approximate method for solving the complete system of equations of chemical kinetics.

The proposed method is based on a physically reasonable assumption that equilibrium in the bimolecular reactions is established much faster than the full chemical equilibrium, being applicable when this assumption holds. The method includes only one differential equation for calculating the change in the number of molecules per unit mass of the mixture due to the reactions of recombination and dissociation. This equation is used instead of dozens of equations of chemical kinetics. In the present work, we propose to supplement this equation with an algebraic equations for calculating the equilibrium composition at given values of the density, molar mass and internal energy or temperature. The equations are derived based on the characteristic function (entropy or Helmholtz free energy) extremum method.

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ATOMISTIC SIMULATION OF DETONATION INITIATION IN AB MODEL OF ENERGETIC MATERIAL

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Evolution of an ultra-short shock wave (SW), generated by a femtosecond laser pulse in a metal film with micrometer thickness, can be studied in details using molecular dynamics (MD) simulation, in which trajectories of all atoms of a sample are calculated during several nanoseconds. Such modeling gives full information about generation and evolution of SW from atomic scale and can be used for analysis of experimental data, as well as for planning experimental research aiming for a study of specific response of condense-phase explosives to impact loading. Large-scale MD simulation of detonation initiation in an unbounded thin film of condense-phase explosive uniaxially compressed by an ultra-short SW driven by a potential piston is performed. Interatomic forces and chemical reactions in the explosive are represented by AB model [1, 2] using the simplified REBO potential. Variation of piston velocity and loading time gives a 2D region

of velocity-time parameters, where transition of SW to detonation wave is observed. On completion of loading time the piston is removed from simulation, thereby the sample boundary becomes free, which leads to generation of an unloading wave, similar to what happens after irradiation of metal film by a femtosecond laser pulse. The point (P,V) on Hugoniot corresponding to picosecond initiation of combustion for the given AB explosive makes it possible to estimate the highest speed of piston v_{p0} for which detonation cannot be generated by ultra-short pulse loading. From data [2] we obtain an estimate of the critical piston speed of $v_{p0} \approx 2.77$ km/s, which agrees with our simulation. Analysis of evolution of calculated pressure profiles gives a critical thickness of such AB explosive film, which is required for transition from SW to detonation wave. Introduction of cylindrical pores into samples at small enough depths decreases the critical velocity-time parameters for transition to detonation.

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HYDRODYNAMIC INSTABILITY AT THE INTERACTION BETWEEN SOUND AND DIFFUSION FLAME

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This paper presents results of experimental studies of the effect of external acoustic perturbations on the stability of the diffusion flame and gas jets. Depending on the rate of fuel supply two types of flame have been experimentally simulated - attached and detached flame. It was found that under acoustic influence the sinusoidal mode of instability arises at initial distance of jet. As the distance downstream the oscillations grows up. It leads to fragmentation of the jet into two vortex streets. Inside the jet under the acoustic influence two counter-rotating vortices arises. The main effect caused by turbulization of combustion zone is the flame surface increase that leads to the strengthening of the leading combustion processes such as thermal conductivity and diffusion, the further development of turbulence and, as a result, a significant acceleration of the flame.

The criterion of gas jet bifurcation was found. Threshold frequency of acoustic impact is linked with the characteristics of the jet (jet velocity and diameter, as well as the physical properties of the gas jet).

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COUNTER INFLUENCE OF HALOALKANES ON CONDENSATION AND COMBUSTION OF ACETYLENE

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Influence of haloakanes on combustion development is a scientific problem of permanent interest due to their wide use in fire extinguishing and recent reports on their promoting activity in particular conditions [1] [2]. Acetylene detonation control is an actual task regarding safety and new energetic technologies development.

In present work an influence of CF_3H and CCl_4 on the ignition of 3.5-20%($2C_2H_2$+$5O_2$)+Ar mixtures were investigated in the shock tube of a standard design with inner diameter 50 mm at pressures 1.5-3.0 bar and temperatures 950–1400 K. Several calibrated piezoelectric gauges allowed to determine the incident shock wave velocity used for calculation of "frozen" parameters of the flow. In preliminary experiments the time-resolved spectra of combustion region were obtained using high-speed ICCD camera LaVision. Subsequently OH radical emission signal was used for induction time measurement, and emission-absorption diagnostic at Na line 589 nm—for pilot temperature measurements.

In contrast to previously studied condensation detonation of acetylene [1], the ignition of acetylene-oxygen mixtures was significantly decelerated in presence of CCl_4 admixture. CF_3H demonstrated minor inhibiting activity.

ChemKin software package and a modern comprehensive kinetic mechanism of acetylene oxidation [3] were used for numerical modeling of combustion development. Consideration of reaction involving studied haloalkanes and active radicals provided a good agreement between experimental and modeled results. During the next stage of work the experiments in highly enriched mixtures were carried out providing important information about acetylene condensation detonation limits in presence of minor amount of oxygen.

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PROMOTION OF METHANE IGNITION BY HALOGEN- AND PHOSPHORUS-CONTAINING ADDITIVES

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Chemically active halogen- and phosphorus- containing additives are usually considered as combustion inhibitors [1], and are widely used in fire extinguishing. Impact of phosphorus-containing species on combustion processes is also well studied due to their high efficiency of inhibition and their promising application as an alternative to halons [2]. However recently it was reported of the promoting action of these additives on ignition of methane at the increased temperatures [3] [4]. These effects can have a great practical importance for development of the diesel engines working at gaseous methane, and also for the SCRAMJET.

In this work the experimental and numerical study of promotion of spontaneous ignition of methane-oxygen mixtures by the additives of CF_3H, CCl_4 and $(CH_3O)_3PO$ at various initial temperatures has been carried out. It is shown that efficiency of promotion by halon additives significantly grows with fall of temperature and increases with the concentration of an additive. CCl_4 has the most effective promoting effect at a temperature of 1400 K and the time delays of spontaneous ignition of mixture of $20\%(CH_4+2O_2)+Ar$ are reduced more than by 10 times at addition of 3% of CCl_4. Efficiency of promotion by $(CH_3O)_3PO$ monotonously falls with growth of initial temperature, remaining rather high in all range of temperatures (1400–1800 K).

The numerical kinetic analysis of the obtained results has shown that the main mechanism of a promotion of ignition by halogen containing species consists in reactions of active radicals (Cl, CF_2), formed at dissoci-

ation of the molecules of additives, with initial molecules of CH_4 and O_2, which results in initiation of the chain reactions of ignition. The mechanism of a promotion of spontaneous ignition of methane -oxygen mixtures by the $(CH_3O)_3PO$ consists in formation of OH radicals a result of interaction of a $(CH_3O)_3PO$ and the products of its destruction with oxygen.

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ENERGY GAIN AT PYROLYSIS AND COMBUSTION OF METHANE–ACETYLENE MIXTURES

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In the previous works [1, 2] the possibility of use of energy of carbon condensation at detonation decomposition of acetylene for development of environmentally friendly power set-up is considered. However acetylene is not natural fuel and its production demands additional power and economic expenses. Therefore studying of possibility of elaboration a united power cycle where the natural gas methane as initial fuel will be used is very actual, and the main energy release will occur not at the direct oxidation of methane, and at the allocation of energy of condensation of carbon and combustion of hydrogen which are formed at the thermal decomposition of methane.

In this work the energetics of the complex cycle including the partial oxidation of methane providing heating and conversion of a mixture to hydrogen and carbon vapor and the subsequent stages of process - a heat release at carbon condensation, separation of the condensed particles and hydrogen combustion are analyzed. The optimum regimes of such cycle providing the minimum yield of carbon dioxide and the maximum power efficiency of the subsequent processes of condensation and hydrogen combustion are determined. Comparison of absolute amount of the energy developed on 1 mole of fuel mixture at traditional combustion of methane-air mixture and at the proposed power cycle and also at detonation pyrolysis of acetylene is carried out. The quantity of a valuable industrial product

- the carbon nanoparticles which are formed at generation of 1 MW of thermal energy is evaluated.

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CHEMICAL IONIZATION DURING OXIDATION OF ACETYLENE AND METHANE MIXTURES: SHOCK TUBE AND MODELING STUDY

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The phenomenon of chemical ionization in flames, that is, the formation of ions via chemical reactions between electroneutral substances, was discovered in the late 1940s. The electrical nature of flames has long been realized. The high levels of ions of non-thermal origin in the reaction zone of flames was an evidence of chemi-ionization. It was experimentally demonstrated that a hydrocarbon fuel was needed for chemical ionization, and shock tube experiments have additionally demonstrated that oxygen should be present. Consequently, it was accepted that HCO+ was the major primary ion. At the same time, there is an obvious lack of kinetic data obtained in shock tubes under conditions such that there are no problems arising from complicated gas dynamics, transfer limitations, or temperature gradients. These data are needed to establish systematic correlations between combustion and ionization, which are expected to be of great practical significance. However, use of shock wave techniques is also impeded by the absence of diagnostic methods for studying ionization kinetics. The choice of methods applicable to kinetic studies in shock waves is quite limited.

This work presents the results of measurements of the concentration of free electrons by a microwave interferometer and by an electric probe during the oxidation of acetylene and methane mixtures behind reflected shock waves. The detailed kinetic model of chemical ionization was constructed based on soot formation kinetic model. The results of detailed

kinetic modeling are in good agreement with the experimental data.

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SHOCK WAVE INITIATION OF AUTOIGNITION OF HYDROGEN–AIR MIXTURES

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Problems related to the autoignition of hydrogen-air mixtures are highly important for operation safety of nuclear reactors and for hydrogen energetics. In spite of extensive studies in this area, there are still many problems directly concerned with the ignition delay times of H_2/O_2 mixtures and with the conditions under which these processes occur. In the current work, experimental spectroscopic measurements of the ignition delay times were carried out. The ignition delay times were determined from the optical absorption of hydroxyl radicals in the ground state (λ = 306.8 nm) and from the emission (λ= 308 nm) of electronically excited hydroxyl radicals $\dot{OH}$. The experiments were performed with $1.5\%H_2$ + $1.5\%O_2$ + Ar mixtures in the temperature range 960 -1670 K at a pressure of p = 1 bar. The level of possible impurities was checked by monitoring the emissions of electronically excited $CH^{\star}$ (λ = 429 nm), $C_2^{\star}$ (λ= 516.5 nm), and $CO_2^{\star}$ (λ= 363 nm). To extend the range of low-temperature measurements, the promotion of the autoignition of H_2/O_2 mixtures by additives of oxygen atoms in an amount of 80±20 ppm was used. The numerical modeling of our own experimental results and the available literature data on the ignition delays of hydrogen-air mixtures made it possible to describe the shock tube measurements of ignition delays within the framework of a generalized kinetic mechanism over a temperature range of 950 to 2500 K at pressures from 0.6 to 80 bar.

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THE ROLE OF RADIANT PREHEATING OF THE FRESH FUEL IN FLAME ACCELERATION IN DIFFERENT GASEOUS MIXTURES

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The paper studies the flame propagation through the reacting gas-suspension of combustible gaseous mixture and suspended inert solid micro particles. The particles, suspended in the gaseous mixture ahead the flame front, absorb the radiant heat flux out from the hot combustion products and transfer it to the gaseous mixture by means of molecular and convective thermal conduction. It is shown that in case of highly reactive mixtures such as hydrogen-oxygen this phenomenon causes modest (not greater than 10 percents) flame acceleration in case of uniform particles distribution. The origin of flame acceleration in this case is the preheating of the fresh fuel ahead of the flame front, limited by the burning velocity. The temperature increase is proportional to the heat flux from the flame surface (σT_b^4, where T_b is the temperature of burning products) and inversely proportional to the burning velocity. In hydrogen-air mixture the burning velocity diminishes compare with the hydrogen-oxygen case as well as the heat flux. As a result the rate of preheating rises and the corresponding burning velocity increase reaches 30 percents. In the hydrocarbon-air mixtures the T_b value is not sufficiently lower than in the hydrogen-air one, on the other hand the burning velocity changes by the order. It results in the relatively high preheating of the fresh fuel adjacent to the flame front (up to the 1000K) that in turn causes the changes in flame propagation mechanism and corresponding sufficient flame acceleration. On the other hand in case of sufficiently non-uniform distribution of the particles the radiant volumetric heating may be resulted in forming the local ignition kernels inside the clouds of suspended particles far ahead of the flame front. In this case there is almost no gasdynamical interaction between the flame front and the preheating zone and such conditions can be treated as a case of zero burning velocity.

MODES OF CHOCKED FLAME INSTABILITY DEFINED BY THE PECULIARITIES OF COMBUSTION KINETICS AT RISING PRESSURE

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The dynamics of combustion wave depends on the large number of factors of different physical and chemical nature that complicates setting the experiment and interpreting its results. For today a wide variety of experimental data is accumulated for different cases of accelerating flame evolution, including the deflagration-to-detonation transition, onset of the so-called chocked flames, quasi detonations, slow detonations etc. One should expect similar physical origins of all the possible transonic and supersonic combustion regimes as they arise in the quite close conditions: first the flame accelerates in the flow like a piston-driven one and then achieves the transonic chocked regime, which further evolution in some cases can provide the onset of the detonation. The aim of the paper was to analyze the structure and the stability of the chocked flames to understand the origins of different possible combustion modes. The numerical solution showed that the chocked flame structure was as follows: the compression waves irradiated from the reaction zone were chocked by the locally supersonic flow on the flame tip and started to compress the mixture inside the flame front. At the same time the flame front propagating with the subsonic speed relatively to the moving fresh mixture acted like a piston and the compression of the mixture ahead of the flame front continued. Therefore further flame evolution was determined by two mechanisms: 1) compression of the fresh mixture and 2) compression of the mixture inside the reaction zone. The first mechanism provides burning velocity increase, the second one can either accelerate or decelerate reaction depending on the pressure-dependent reaction behavior in the observed pressure range. The competition of the mentioned mechanisms determine the further flame dynamics: i) the flame speed saturates and one can observe quasi-stable supersonic flame or as it sometimes called "quasi detonation", ii) the flame accelerates and transition to detonation takes place, iii) the chocked flame decays transforming into the subsonic deflagration wave.

FLAMES AND DETONATIONS INSIDE OBSTRUCTED CHANNELS AND GAS-LADEN COMBUSTIBLE MIXTURES

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For decades clear understanding of the non-steady and transient regimes of gaseous combustion remained to be a topical problem of the combustion theory as it was important for the explosion safety and propulsion systems design. However, in spite of wide range of experimental data there is still no systematic analysis of the studied phenomena. The aim of the paper was to resolve the features of the unsteady flames propagating through gaseous combustible mixtures in different external conditions intrinsic to the real technical system environment. To understand the roles of surface and volumetric effects we considered flames propagating through smooth and obstructed channels filled with gaseous and gas-laden combustible mixtures. It was found that the leading role in the flame evolution including its acceleration and transformation into the detonation belongs to the compression waves irradiated out from the reaction zone. The compression waves interference and interaction with the flame front and the flow define the peculiarities of flame evolution on the different stages of its acceleration. Channel walls and other large scale obstacles determine the evolution of the flame front via the diffraction and refraction of the compression waves that can cause either acceleration or stabilization of the flame. The suspended micro-particles act on the sufficiently smaller spatial scales absorbing volumetric momentum and energy and decreasing the intensities of the travelling compression waves and the flame acceleration. The overall pattern of the energy redistribution on the different spatial scales obtained in this paper should be taken into account while estimating hazardous impact of gaseous explosions.

QUANTITATIVE CRITERIA FOR COMPOSITION OF HYDROGEN BASED MIXTURES FOR USE IN SPARK-IGNITION ENGINES

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The use of hydrogen as a fuel in spark-ignition engines becomes a topical problem nowadays due to the possibility of hydrogen generation by renewable energy sources. However, low detonability limit of hydrogen could lead to detonation while burning, what, in its turn, could lead to rapid destruction of combustion chamber and reduction of its working lifespan. Therefore, in the present paper we investigate the method aimed to increase hydrogen detonability limit, consisting in the use of small additions of less energetic substances to basic hydrogen–air mixture. Among these substances we chose: (i) methane, (ii) steam, (iii) air excess (lean hydrogen–air mixtures). Numerical simulation of combustion was carried out with the usage of gasdynamics model and detailed chemical kinetics mechanism [1]. Combustion modeling of mixtures with different quantities of additions in engine chamber with typical parameters (compression ratio 11.4, engine speed 1500 rpm, displacement 1.7 L, spark timing 10°CA before TDC) showed that mixtures with substitution of 1.0% (vol.), 2.0% and 3.0% of hydrogen and more in stoichiometric hydrogen–air mixture by methane, steam and air excess correspondingly provide nondetonative regime of burning. The increase of additions quantities (reduction of substituted hydrogen) results in decrease of engine efficiency, characterized by decrease of maximum in-cylinder pressure and increase of timing at which maximum pressure is observed. We mean the combustion regime with maximum in-cylinder pressure less than 8 MPa and its corresponding crankshaft angle no more than 20°CA by optimal regime. According to this convention we found that following quantities of additions provide optimal combustion: (2.5–3.0)% of methane, (3.1–5.4)% of steam, and (4.2–7.3)% of air excess. These results demonstrate that methane reduces combustion intensity more strongly than steam or air excess. Analysis of chemical conversion indicated that this behavior is due to oxygen deficiency when burning mixtures with methane as compared to mixtures with steam.

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GAS MONITORING SYSTEM FOR NUCLEAR POWER PLANTS AND HYDROGEN FACILITIES

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Safety systems and mitigation concepts for nuclear power plants, hydrogen fuelling stations and hydrogen infrastructure requires detailed data on hydrogen concentration in a case of hydrogen leakage. The objective of the present work is to develop gas monitoring system for hydrogen detection. Not only hydrogen, but oxygen, steam and other components concentrations are important for safety analyses. Hydrogen sensors should be accurate, sensitive, and specific, as well as resistant to long term drift and varying environmental conditions. Presented gas detection system consists of two parts: first for continuous monitoring of concentrations under normal ambient conditions and second for temporary monitoring under elevated ambient temperatures and pressures during possible accident. The system determines high hydrogen concentration (5-90%) under 1-5 atm. pressure, relative humidity up to 100% and ambient temperatures up to 240°C.

PRECHAMBER INITIATION OF GASEOUS DETONATION IN A CHANNEL

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Prechambers of greater diameter are usually used as a method of steady detonation initiation for studies of the detonation propagation in the connected channel [1]. It was obtained that a prolongation in time of the source of ignition has to be taken into account for evaluation of the energy of the direct initiation of detonation [2].

A process of deflagration-to-detonation transition in propane-butane-oxygen and acetylene-oxygen mixtures, in an open channel with a circular cross section with a diameter of 3 mm, was investigated experimentally. Detonation initiation was carried out by burning the mixture in the prechamber connected to the channel. The prechamber was considered as an extended source for the initiation of the detonation of a finite volume.

To determine the boundary conditions at the entrance to the channel, a piezoelectric pressure transducer was used. To measure the velocity of a flame front, photodiodes, installed along the axis of the channel, were used.

The influence of the dimensions of the prechamber, equivalence ratio and fuel on the pressure profile, and evolution of the flame front along the axis of the channel are presented. It was shown that, the dynamics of the flame front and shock waves in the channel can occur in different scenarios depending on the geometry of the prechamber and equivalence ratio: the push-effect of the prechamber due to the spreading of the combustion products, the combined effect of the combustion products and compression waves, or direct detonation formation.

The pre-detonation distances and the minimal energy of direct initiation of the detonation were determined. The experimental map of the possibility of direct detonation initiation depending on the volume of the prechamber or the energy released in the prechamber and ER for propane-butane and acetylene-oxygen mixtures is presented.

The work was supported by the RFBR N-13-08-01227-a and RAS (Combustion and Explosion).

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DIRECT INITIATION OF A HYDROGEN–AIR MIXTURE DETONATION

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The report presents the results of an experimental study of the direct initiation of spherical detonation of a near stoichiometric hydrogen–air mixtures. Combustible mixture was inside a thin rubber spherical envelope. The volume of the mixture was about 7 m^3. There was a measuring bar inside the envelope at which PCB pulse pressure sensors, ionization detectors, and a triggering device were placed. The rubber envelope with the combustible mixture was located inside 13Ya3 explosion chamber 12 m in diameter. The data show that the pressure in front of a spherical explosion wave is initially reduced to a value below the Chapman-Jouguet pressure

and then increases and at a distance of about 1 m reaches a stationary value.

INVESTIGATION OF THE EFFECT OF THE EJECTOR ON THE PERFORMANCE OF THE PULSE DETONATION

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One of the promising low-thrust engines is the pulse detonation engine (PDE). This is accounted for by the fact that the heat efficiency of the fuel burned in a detonation wave exceeds the efficiency of the fuel burned at a constant pressure by 13 % [1]. One such way of enhancing the engine thrust is use of an ejector. It is shown that the use of an ejector in an engine with a constant flow rate can result in a gain in the thrust as high as about 35 % [2] and about 50 % [3]. In [4] it is shown that use of an ejector in the pulse engine may result in a gain in the thrust to 100 %, however.

The purpose of this work was to determine the dynamics of the thrust in a pulse detonation engine fitted with an ejector during some successive pulses and also to show the dynamics of the ejected ambient air flow rate.

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FORMATION OF THE OVERDRIVEN DETONATION WAVE IN THE FLOW OF METHANE–OXYGEN MIXTURES IN THE CHANNEL OF VARIABLE CROSS SECTION

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Formation of the overdriven detonation wave in methane-oxygen mixtures in the channel was experimentally investigated. To create an overdriven detonation wave the decay of the stationary detonation into the shock wave and the flame front was implemented in the transition to a larger channel cross-section [1]. This is accompanied by an increase in pressure in the unreacted mixture ahead of a traveling shock wave [2].

Ignition of the mixture was carried out by a spark gap, located on the end of the combustion chamber. Thus, the created complex of the shock wave and the flame front moving behind him propagated in the channel with a conical narrowing. At the exit of the conical constriction formation of the overdriven detonation wave recorded with the parameters several times greater than the parameters of the stationary Chapman-Jouguet detonation. Excess of pressure compared to the stationary Chapman-Jouguet detonation was up to three times. The velocity and pressure of the detonation wave were determined depending on the the composition of the mixture. Detonation cell sizes, diagrams of compression waves and flame front propagation in the combustion chamber depending on the mixture composition are presented.

The work was supported by the RFBR N-13-08-01227-a and RAS (Combustion and Explosion).

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INVESTIGATION OF DEFLAGRATION TO DETONATION TRANSITION IN SPIRAL CHANNELS

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One of the primary targets of detonation applications is run-up distance reducing. It decreases the amount of combustible mixture which burns in ineffective (not detonation) mode. It is well known that temperature rise in reflected from obstacles and channel bends pressure waves accelerates the transition to detonation. Nevertheless extreme amount of bends and obstacles may inhibit DDT or decouple detonation wave either.

Present work concerns investigation of deflargration to detonation transition in gaseous combustible mixtures in spiral channels. Authors use an Archimedes's screw to split the detonation tube on two spiral channels of half-disk cross-section.

Flame speed velocity along the channel and the point of deflagration to detonation transition was experimentally investigated. Self-radiation of flame and pressure profiles was measured by pairs in four sections along the channel. Experiments was made with hydrogen-oxygen and methane-oxygen mixtures in spiral channels of half-circle cross-section and straight channel of circle cross-section.

THE EMISSION SPECTRA OF LOW-INTENSITY SHOCK WAVES PROPAGATING IN He DILUTED WITH Xe

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Propagation of shock waves in helium, diluted a small admixture of xenon ([Xe] = 0.1–10 %), experimentally investigated in a high-vacuum shock tube "Yashma" (residual pressure of gas $P < 10^{-6}$ mbar) in the next regimes: the shock wave Mach number M = 2.3–3.3, the equilibrium pressure and temperature behind the shock front P = 0.3–0.7 bar, T = 850–1350 K. The highly purified gases were used. The spectra measurement was performed from the shock tube end. Were applied the spectrograph ACTON 2150 (Princeton Instrument) and high speed CCD-camera LeGa-3, equipped with the intensifier based on the electro-optical transducer,

sensitive in the range of 115–900 nm. Were measured the emission spectra in the range from 180 to 650 nm. The data were obtained on the dependence of the spectra on the concentration of Xe, the initial thermodynamic parameters of gas mixtures and the rate of shock waves. The optical transitions lines in Xe are Identified. It has been shown that a decrease in the concentration of Xe in the mixture causes the shift in the emission spectrum toward the vacuum ultraviolet region.

The work is supported by the Program of the Presidium of RAS "Matter under High Energy Densities".

EXPERIMENTAL STUDY OF INTERACTION OF Cl-ATOMS WITH THE MOLECULES C_2H_2 BEHIND SHOCK WAVES

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The halogenated hydrocarbons are considered a species that may prevent the explosion and detonation of methane-air, hydrogen-air and othercombustible mixtures (CCl_4 [1], CF_3H [2]). However, under certain conditions (particularly at elevated temperatures) halogenated species do not inhibit combustion they may even accelerate the ignition of hydrocarbon-oxygen mixtures (Cl_2 [3], CCl_4 [1], CF_3H [4]). Such effects could be explained by the interaction of the products of admixture pyrolysis with the initial compounds, resulting in the acceleration of active radical formation during the induction time [5]. In contrast to other hydrocarbons, acetylene self-ignition and detonation can happen spontaneously without an oxidant. Typically, self-ignition and detonation of acetylene occur most easily and rapidly at elevated pressures [6-7]. Thus, investigation into the methods of inhibition of acetylene detonation is of great importance. However, the kinetics of in uence of halogenated species on the acetylene detonation process remains unexplored.

The goal of the present work was to study the influence of atoms Cl, as product of dissociation of CCl_4, on the kinetics of acetylene decomposition behind shock waves. Using the method of atomic resonance absorption spectroscopy (ARAS) at the resonance line Cl(I) at 139.97 nm the change of the concentration chlorine atoms was investigated in various mixtures $CCl_4 + C_2H_2 + Ar$ behind shock waves at temperatures of 1000-3000 K and pressures of 1-16 bar. The experimental results are compared with a kinetic modeling of the thermal decomposition of acetylene and its re-

actions with chlorine atoms at different temperatures and pressures using Chemkin-4. This work has been supported by grant RSF 14-19-00025.

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THE STUDY OF KINETICS CF_2 RADICAL FORMATION AT THE PYROLYSIS OF CF_3H BEHIND SHOCK WAVES

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Various halogenated hydrocarbons are widely used for the fire fighting [1-4] Trifluoromethane is considered to be one of the most promising inhibiting additives to methane-air, hydrogen-air and other gas mixtures [2].Combustion suppression efficiency occurs not only from its endotermicy during pyrolysis, when the temperature of mixture decreases rapidly, but also due to chemical inhibition of chain combustion reactions [2-3] It is assumed that CF_2,is a primary product of trifluoromethane dissociation and is responsible for the suppression of the chain reactions of combustion. However, as it was shown in the papers [4], under certain conditions, such additive is not only inhibits the combustion and can even accelerate the ignition of the hydrocarbon-oxygen mixtures. Therefore, for possible practical application of CF_3H as an inhibitor additive it is necessary to study the kinetics of CF_2 radical formation at the pyrolysis CF_3H in a wide range of temperatures, pressures and concentrations of initial components. The study of the kinetics CF_2 radical formation using the method Molecular Resonance Absorption Spectroscopy (MRAS) were performed behind shock waves in UV range at a wavelength λ=251.9 nm. More than 80 successful experiments in the temperatures range of 1180$\leq$ T5$\leq$ 2780 K and pressures 1.5$\leq$P5$\leq$16 Bar behind reflected shock waves were carried out. The initial concentration of CF_3H in argon was varied from 0.0038 to 2.7%. As a source of radiation line of CF_2 radical

the microwave discharge lamp with the mixture of 1% CF_3H in He at the pressure of 6 mbar was used. From the experimental data the temperature dependencies of the equilibrium constant and the dissociation rate constant of CF_3H were determined at different pressures. The experimental results are compared with the kinetic modeling of the thermal decomposition of CF_3H at different temperatures and pressures using Chemkin-4.

This work has been supported by grant RSF 14-19-00025

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NUMERICAL STUDY OF THE GAS FLOW IN THE NOZZLE AND A SUPERSONIC JET FOR DIFFERENT VALUES OF SPECIFIC HEATS

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On the basis numerical modeling the process has been investigated of the expiration of a supersonic jet from a flat nozzle for two ratioes of specific heats and different parameters NPR. This parameters represents the ratio of the pressure at the nozzle inlet to the pressure in the environment. As a result the solid state grid model have been created for the numerical simulations of the flow of gas inside the nozzle and jet formation of compressed gas from the nozzle, which can be used to analyze the data structure.

The calculation have been carried out for values of specific heats Cp/Cv = 1.4 and Cp/Cv = 1.3, the value of the parameter NPR being 20, 15, 10, 5. When the parameter NPR = 20 there is a structure that is typical for regular reflection with the intersection point on the axis located at the exit of nozzle. When reducing to 10 NPR the structure resembling the regular reflection remains however it is shifted into the nozzle, the flow separation occurs. With further decrease of NPR to 5 the number of consecutive normal shock waves in the nozzle increases. Subsonic separating zones appear. This mode is preceded by the formation of Mach reflection. Note

that for the same value of the parameter NPR, but at a smaller value of Cp/Cv intersection point shifts further away from the inlet section of the nozzle. The flow separation becames substationally less.

THREE-SHOCK EFFECT OF THE APPEARANCE OF CONFIGURATIONS WITH A NEGATIVE ANGLE OF REFLECTION ON THE STRUCTURE OF A SUPERSONIC JET

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The expiration of the supersonic jet from a nozzle at off-design operation occurs when the pressure in the gas stream at the nozzle exit is different from the ambient pressure medium. There may be cases of over-expanded $P_1 < P_a$ and under expanded jet, i.e. $P_1 > P_a$ (P_1 – the gas pressure in the output section of the nozzle, P_a – pressure in the external environment). As a result, systems of alternating expansion and contraction waves and shocks appear inside the jet which may have a different configuration. There may be a three-shock configuration with a negative angle of reflection [1]. If the reflected wave in this configuration, crosses the line of symmetry, it is clear that such a configuration can not be stable, on the line the gas begins to accumulate, stationary process flow will be disrupted.

One can expect new wave structures of supersonic jet to appeare or even the occurrence of vibration modes. In any case, the occurrence of a triple shock configuration with negative angle would lead to the change in the mode of operation of rocket engine. This effect is real to the expiration of jets from the nozzles, since the products of combustion of conventional fuels have a fairly low ratio of specific heats.

In the report the analytical studies with the aim of three shock theory are presented of different forms of three-shock configurations that may occur at the nozzle exit. They have been obtained over a wide range of governing parameters: pressure drop across the oblique waves emanating from the nozzle exit, the ratio of specific heats and the Mach numbers.

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NUMERICAL SIMULATION OF AEROGASDYNAMICS OF A FLIGHT VEHICLE WITH A HYPERSONIC LIQUID-FUEL RAMJET

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A key phase in creation of a real flight vehicle with a hypersonic liquid-fuel ramjet is a procedure used to form its aerogasdynamic arrangement. To reduce the number of expensive physical experiments it is worth conducting the virtual computational experiments with math simulation.

The paper provides an aerogasthermodynamic scheme of a flight vehicle with a hypersonic liquid-fuel ramjet developed with Navier-Stokes equations in the CFD package. The combined aerogasdynamic engineering of the flight vehicle and the hypersonic liquid-fuel ramjet using supercomputational hardware and computational experiments with a simulation math model allows us: • to form aerogasdynamic arrangement of the flight vehicle with the hypersonic liquid-fuel ramjet capable to maneuver within the Mach number from 6 to 8 at an altitude from 20 km to 30 km; • to demonstrate that a specific impulse from 10 to 14 km/s (1000–1400 s) can be reached at completeness of combustion more than 85%, if a pure or mixed hydrocarbon fuel is volumetrically fed in the supersonic flow inside the combustion chamber; • to show that in the above flight conditions at an attack angle from 6° to 8° a small flight vehicle consumes no more than 0.7 kg/s of liquid hydrocarbon fuel; • to illustrate that allowance for the radiation of gas and walls in the math model does not markedly change the gasdynamic processes in the hypersonic liquid-fuel ramjet passage and its integral characteristics.

More over, it is noted that intake of the outboard air through a punched or porous surface of the hypersonic liquid-fuel ramjet nozzle permits us: • to control the vehicle flight within the above ranges of altitude and speed by affecting the hypersonic flow in the nozzle; • to increase hypersonic liquid-fuel ramjet specific impulse; • to reduce the convective heat flows to the nozzle walls and bottom of the flight vehicle.

An evaluative heat analysis of the flight vehicle with the hypersonic liquid-fuel ramjet is made on which basis: • typical temperature regimes of the flight vehicle body are defined and thermal protection for the key components are selected; • it is detected that the combustion chamber can be thermally protected with active cooling with fuel while it is heated up.

NUMERICAL SIMULATION OF THE HIGH-ALTITUDE HYPERSONIC FLOW OF A BODY UNDER SHOCK-WAVE INTERACTION

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The paper considers problems of simulation of interaction of the fourth-type waves typical for the high-altitude hypersonic flow of flight vehicles.

The key target of the paper is to identify the most effective and promising numerical methods for the considered area of problems.

The complete validation of a method asks for a huge amount of work, to simplify the task the paper considers 2D axisymmetric problems of flow without separation on the windward side of blunted bodies.

Three cases are selected: • the ONERA experiment on hypersonic flow of a cylinder under the shock-wave interaction in front of it with incident shock [1], • reproduced data of the OREX flight vehicle for a point of its trajectory at H = 92.4 km [2], • the hypersonic flow of a two-component cone with a separated-flow region at the interface [3].

The math methods are based on the widely used numerical schemes: • DSMC–Monte-Carlo simulation (direct statistical simulation) implemented with the SMILE software, • method of finite volumes (AUSM+ scheme)—Godunov-type method implemented with the ANSYS Fluent software, • method of finite volumes (Kurganov–Tadmor scheme)—central-upwind scheme implemented with the OpenFOAM software.

A series of calculations using the above methods are made for each case. Upon analysis of the results conclusions are drawn on applicability of a numerical method to settle problems of this type. In particular, the Kurganov–Tadmor scheme combines high accuracy and low computational cost, is good for the engineering analyses. While the DSMC with its practically unlimited accuracy is good for academic research.

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EXPERIMENTAL INVESTIGATION OF SHOCK WAVE–BOUNDARY LAYER INTERACTION INSTABILITY

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As instability caused by Shock Wave–Boundary layer interaction can lead to serious control issues [1], it is a subject of investigation. It was discovered that unsteady behavior of separation bubble contains the low frequencies fluctuations [2]. Current work is devoted to the investigation of the instabilities caused by interaction of shock wave with turbulent boundary layer on the heated ramp surface.

By means of PIV detailed flow structure of separation and reattachment regions for the case of 30°ramp angle were measured. For the evaluation of the surface heating influence the ratio of wall temperature towards outer flow temperature T_w/T_∞ in the experiments was varied in the range from 1.8 (adiabatic conditions) to ∼3. Average velocity fields for temperature ratios of 2.77 and 3.11 have shown regions of reverse flow (separation bubble), and velocity in this region reaches $\sim 0.1U_\infty$. The averaged velocity profiles of the reattached boundary layer shows that rising of temperature ratio leads to the increase of boundary layer recovery length from 4.6 mm for adiabatic case to 11 mm for $T_w/T_\infty = 3.11$. In order to study fluctuations of separation bubble statistical analysis was applied. According to the POD analysis about 60% of whole energy is stored in the first 5 spatial modes. The first 2 modes represent pulsation of separation region. In case of ramp with temperature ratio of $T_w/T_\infty = 2.77$ and 3.11 first spatial mode contains almost 40% of energy meanwhile in case of adiabatic surface the amount of the energy stored in the first mode is 15%. It is obvious that elevation of surface temperature leads to redistribution of energy stored in spatial modes represented separation region motion. RMS velocity fields also have shown amplification of separation buble fluctuations with surface heating. Velocity fluctuation near separation and reattachment points reaches $0.38U_\infty$.

It was shown that increase of temperature ratio affects both incomming and reattached boundary layer and amplifies separation bubble motion.

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RAYLEIGH–TAYLOR AND RICHTMAYER–MESHKOV INSTABILITY OF NEWTONIAN SUBSTANCE AT HIGH ENERGY DENSITIES

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A series of experiments have been carried out to study the development of the free boundary instability of thin layer of water with a thickness of 1 mm due to impact of the unsteady shock wave. Nonstationary damped shock wave (Taylor's wave) was created in the water layer by evaporation of a thin (about 10 microns) target, located on the bottom surface of the layer of water. This evaporation occurs under a pulse of laser radiation with a wavelength of 532 nm, energy 0.35 J and pulse duration ∼10 ns. The pressure on the Taylor's wave front equals to 80 MPa according to the calculated estimates. Dependencies of particle velocities on time $V(t)$ have been obtained in the experiments using PDV method. It can be seen that at each time from the beginning there is a whole set of values of velocities. So we can assume that the speed of different dispersed microdroplets of water is recorded almost simultaneously. These microdroplets of water move at different speeds and were caught by the beam spot of erbium laser. Theoretical part consists of a numerical study of the turbulent stage of development of the Rayleigh–Taylor instability for viscous media with different material rheology for high density. When the lead plate collides with another plate of light metal at high-speed, metals are transformed in a "fluid state" in some region near the contact surface. At the same moment the lead plate is decelerated from the original speed to a standstill. Loss of the stability of colliding surfaces are accompanied by the characteristic outbursts of light metal in a more heavy metal-lead. These outbursts can be seen on the photo of microsection of this structure. In experimental studies, it cannot be accurately measured their amplitudes due to partial destruction of their peaks. In numerical simulation similar structures were obtained as a result of collision of the lead plate with a thickness of 4 mm with the titanium plate with a thickness of 4 mm at the speed of about 500 m/s. It is believed, at the moment of the collision, that the metals are in a liquid phase with the corresponding density and viscosity.

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NUMERICAL SIMULATION AS IMPORTANT TOOLS IN DEVELOPING NOVEL HYPERSONIC TECHNOLOGIES

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Development of novel hypersonic technologies necessarily requires the development of methods for analyzing a motion of hypervelocity vehicles. This paper could be considered as the initial stage in developing of complex computational model for studying flows around hypervelocity vehicles of arbitrary shape. Essential part of the model is a solution to three-dimensional transport equations for mass, momentum and energy for the medium in the state of both LTE (Local Thermodynamic Equilibrium) and non-LTE. One of the primary requirements to the developed model is the realization on the modern heterogeneous computer systems including both CPU and GPU.

The paper presents the first results on numerical simulation of hypersonic flow. The first problem considered is three-dimensional flow around curved body under angle of attack. The performance of heterogeneous 5 GPU computer system is tested. The second problem highlights the capabilities of the developed model to study heat- and mass transfer problems. Namely, interior heat problem is considered which takes into account ablation of Thermal Protection System (TPS) and variation of the surface shape of the vehicle.

LINE OF ACTION AND ADVANCED SCIENTIFIC TASKS OF THE LABORATORY OF HYPERSONIC AND PLASMA TECHNOLOGY MIPT

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For basic and applied research as well as training in the development of advanced aerospace systems and their power plants under the program 5top100 in MIPT established scientific laboratory hypersonic and plasma technologies (HPT). Lab partners are leading industry and academic institutions, enterprises and aerospace higher education. The objectives of the HPT lab is to conduct fundamental research in gasdynamic flows due hypersonic flow past bodies of different configurations, the determination of thermal properties and characteristics of durability of materials under conditions of high heat loads, the study of hydro-and plasma-chemical processes in high-enthalpy flows, including the polyphase. An important part of the laboratory is to study the integration issues hypersonic aircraft propulsion. The results of some computational and experimental studies of gas-dynamic structure of external and internal flows in a power plant integrated with a hypersonic aircraft. The results of work aimed at forming scientific basis and development of experimental base HPT lab. The outline of the activities of the laboratory in the near and medium term.

SUPERSONIC NOZZLE PROFILING FOR SUPERSONIC AEROSPACE TESTING IN A VIEW OF HIGH-TEMPERATURE OF PROPERTIES OF REAL GASES

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Plasma torches are widely used in manufacturing processes of plasma heating (particularly in supersonic and hypersonic aerodynamical testing), alloys and metal processing (melting, cutting, coating etc.), and also for industrial waste disposal. Current issues of plasma torch modeling are the adequate consideration of MHD-effects in arc currents, intense turbulence generation due to a sharp heat emission (a fluent electric arc zone with the heat density of $2 \cdot 10^{11}$ W/m^3). High temperatures often require both correct transport coefficients and radiation transport calculation in view

of non-equilibrium plasma. Combustion and non-transferred electrical arc heating is often used to expand the available temperature and Mach number ranges of the facilities aimed for aerodynamic testing of supersonic and hypersonic cruise vehicles (HCV) whereas chemical reaction of equilibrium dissociation and ionization take place producing of different multiplicity. These processes are often considered as phase transitions stretched in the temperature scale and resulting in a sharp and non-monotonic variation of the transport coefficients of gas mixtures. In this paper the calculations of certain thermophysical parameters of in the temperature range 260–100000 K basing on the equations of equilibrium dissociation and ionization and in a view of the effects of real gases (4th order virial corrections) and plasma (Debye correction), as well as the comparison of the obtained results with other researchers are presented. The authors also propose a modified technique of one-dimensional nozzle profiling including variable adiabatic index that utilizes the dependence of the gas enthalpy on temperature. According to the results of profiling we developed a supersonic nozzle and to verify the acceleration characteristics of supersonic nozzle, as well as to determine the gas velocity, a series of measurements of stagnation pressure was conducted. As a source of high-enthalpy plasma flow we used a 50 kW plasma torch with a swirl stabilization and expanding channel providing high flow rates, efficient heating of the working medium and small thermal losses in the water-cooled anode surface. Relay on findings, one can conclude that at the vicinity of nozzle exit a transonic flow mode exists that can be preserved at large distances from the nozzle.

SIMULATION OF 3D FLOWS PAST HYPERSONIC VEHICLES IN FLOwVISION SOFTWARE

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Methods for numerical integration of 3D transient Niavier-Stokes equations can be subdivided into two groups: the methods based on using variables velocity-pressure and the methods based on using variables velocity-density. The velocity-pressure methods suit well for simulation of incompressible and low-compressible flows of fluid and gas. Classic methods from this group are not used for simulation of the flows of compressible gas. On the contrary, the velocity-density methods have been developed for solving the problems of super- and hypersonic aerodynamics. However, it is impossible to simulate incompressible flows with neither of these methods.

The first published algorithm for numerical solving the Navier-Stokes equations in variables velocity-pressure was the velocity-pressure split method. Later modifications of this method have been developed, e. g., projection method MAC, methods SIMPLE, SIMPLER, SIMPLEC, PISO. All these methods are based on solving the momentum equation with use of the pressure field and the conservative mass velocities at the cell faces (i. e. the velocities satisfying the continuity equation) obtained at the preceding time step. The velocity field is corrected after solving an additional equation for pressure. The drawback of these methods is that the conservative velocities are calculated at the end of the time step as a result of correction of the velocity field with use of the gradient of the pressure increment. Therefore, these methods cannot be used in a problem with moving boundaries of the computational domain across a fixed (Euler) grid, for instance, due to ablation of TPS.

A new implicit velocity-pressure split method is discussed in the given presentation. The method implies using conservative velocities, obtained at the given time step, for integration of the momentum equation and other convection-diffusion equations. This enables simulation of super- and hypersonic flows with account of motion of solid boundaries. Calculations of known test cases performed in the FlowVision software are demonstrated. It is shown that the method allows one to carry out calculations at high Mach numbers with integration step essentially exceeding the explicit time step.

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ESTIMATION OF RADIATION HEAT FLOWS IN MULTICOMPONENT REACTIVE GAS MEDIUM FOR MODEL DUCT

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Development and improvement of high-technology items of space and aviation technology are necessarily led to increase of specific energy parameters. Moreover reliability and durability requirements increase. Hence requirements for accuracy of conducted calculation also increase at elaboration, designing and creation of new engineering specimens. Present work concerns the question of rising thermal load to construction parts, followed the augmentation of specific energy parameters. The increase of

pressure and temperature at flow paths of engine combustion chambers and propulsion systems bring to rise of specific heat flows, including heat flows of radiant nature. Calculation of radiation heat flows, taking into consideration variety of physic phenomenon for real configuration, represents some computing and physico-mathematical difficulties. Present work contains the comparison of results of radiation heat flows calculation in model duct with uniform cross-section. These results were obtained with use of engineering calculation methods and contemporary computational approaches, which were realized in commercial software. The duct with uniform cross-section was considered as an object. The flow of multicomponent reactive gas medium of combustion products of air-hydrocarbon fuel mixture was examined in that duct at high pressure conditions. It was considered the turbulent flow of multicomponent gas mixture in axisymmetric channel. The combustion process was considered as equilibrium. The wall was considered as temperature with coefficient of radiation, representative all modern structural materials. At calculation with using of engineering methods, given in special literature, which recommended to use in process of creation of aerospace technique specimens, the essential difference in the level of radiation heat flows was determined. This difference can be explained by use of various empirical data, which underlied in engineering methods. As a physical model, used in commercial software, the model of thin radiant layer and discrete ordinate method. The comparison of calculation results has shown the satisfactory correspondence and close magnitudes to one of engineering method. Since the calculation magnitudes of radiation heat flows level may be cause of significant changes of construction, it is necessary to produce enough accurate method of calculation. Such method can be create with use of contemporary physical models and reliable experimental data.

MODELING OF MIXING AND COMBUSTION PROCESSES FOR HIGH-ENTHALPY AIR FLOW AND VARIOUS FUELS

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Modeling of mixing and combustion processes for high-enthalpy air flow and various fuels is a vital task for development of advanced engines for high-velocity aircrafts. When using solid propellants, fuel feed system become more complicated owing to great amount of condensed particles in gas flow mixing with air. Numerical analysis was applied to estimate

the mixing and combustion efficiency for design enhancement. The results of numerical simulation of two-phase flow and air mixing are presented. When using hydrogen as fuel for air-propulsion systems there are various methods to model mixing and combustion. In this work hydrogen mixing, ignition and combustion in high-enthalpy air flow was calculated with kinetic multistage scheme (Dimitrov) for different injection types. Temperature, pressure, velocity and concentration fields, obtained from the computational analysis, allow choosing appropriate fuel feed system.

INVESTIGATION OF POSSIBLE WAYS TO IMPROVE PERFORMANCE OF GDT FOR HIGH ENTHALPY FLOW

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In ground tests of rocket engines (RE), designed to work in the upper atmosphere and space, the problem of the flight conditions simulation arises. The engines of this type have a great nozzle area ratio (ratio of the nozzle exit area to the area of the throat). Therefore, one of the main requirements to the ground tests is maintaining of the unseparated flow in the nozzle of the engine, which can be achieved by various methods. The most cheap and technically simple way is to use gas dynamic tubes (GDT). The figure below shows a scheme of the plant with the GDT.

The basic parameters characterizing the GDT are: the start pressure—the minimum pressure in the combustion chamber of a rocket engine, above which the flow mode in the nozzle transits from the separated to the unseparated, and the stall pressure—the minimum pressure in the RE combustion chamber below which the separated flow forms in the nozzle. Gas dynamic tubes can be used either independently or together with other devices which create a vacuum at the outlet of the GDT (ejectors, exhauster). In this case, the ratio of start or stall pressures to the pressure at the exit of GDT instead of pressures itself should be considered. Also it is necessary to establish minimal start and stall pressures to guarantee the specified cyclogram, and operating conditions of RE. For the considered RE these characteristics are mainly defined by the following geometric parameters: the RE nozzle critical section diameter, the RE nozzle exit diameter, the GTD entry diameter, the GTD throat diameter, the supersonic nozzle length, the length of the GTD inlet diffuser, the length of the GTD throat, the RE nozzle exit angle, and GDT entry angle. In addition,

there is material effect of the nozzle profile shape, and of the combustion products properties (primarily specific heat ratio). In this paper the possible ways of improving the characteristics of GDT are investigated.

Two-dimensional and three-dimensional numerical simulation approaches to unsteady gas flows with various turbulence models have been employed to evaluate the characteristics of the GDT. To confirm the results obtained by numerical simulation, tests employing modeling RE chamber and modeling GDT have been carried out. Comparison of calculated and experimental data has shown the adequacy of the employed simulation methods.

HIGH ENTHALPY HYPERSONIC FLOWS SIMULATION

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Experimental and numerical studies are needed when designing the high-speed engines integrated with the aircraft. Flight experiments are complicated, expensive enough and should be carried out at the final stage of development only. Therefore a large number of studies carried out on the ground facilities. It is necessary to generate the high-enthalpy hypersonic flows, simulating flight conditions. Such flows are characterized by high total temperature and pressure. One of the tasks that need to be solved in the organization of ground research on the facility is the choice of method of heating the working medium. The different heating methods are considered: using the cowper stove or recuperative heat exchanger, adiabatic heating, heating by electric arc or fire heating. Each of these methods has its own advantages and disadvantages. For the experiment it is needed the choice of simulated parameters that depends on the specific tasks formulations. So, for example, it is necessary to simulate the full flow enthalpy and the dynamic pressure to determine the integral engine characteristics. For simulation of processes of ignition and kinetics of chemical reactions necessary to reproduce the static and total temperatures, but this leads to higher enthalpy values. You must also take into account the fact that in ground-based experiments, especially when using fire heater, the working gas composition is different from the pure air that affects the processes of ignition and combustion in the combustion chamber. The fire type heating only allows currently testing of large scale models of aircraft duration of the order of hundreds of seconds with simulated flight conditions with large

Mach numbers. The analysis of different combinations of simultaneously reproduced characteristic parameters is carried out. The numerical flow simulation is important at the design stage. In connection with the increasing power of computer engineering in recent years there was possible the solution of complex simulation tasks on large enough computational grids, containing hundreds millions cells, using modern turbulence models, non-equilibrium chemical kinetics. Before experimental research the preliminary numerical simulation of the flows around aircraft and in the engine duct in the ground facilities conditions in high enthalpy hypersonic flow is performed. The calculated characteristics are determined for following validation. The obtained data allow to predict the expected flight characteristics on the results of ground-based experiments.

ON THE MECHANISMS OF ENERGY DISSIPATION OF GALACTIC COMETS BOMBARDING TERRESTRIAL PLANETS

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It is known [1, 2] that physical mechanisms of energy dissipation for high-speed comets of the Galaxy, which fall on terrestrial planets with no atmosphere and with atmosphere are significantly different. If on planets of the first group (Mercury, Moon and also Mars with a very tenuous atmosphere) galactic comets form large craters with diameters ∼10–100 km, the volume of which is almost proportional to kinetic energy of the comet. Whereas in the atmosphere planets of the second group (Earth and Venus) comet nucleus is destroyed and converted into hypersonic gas jet. When this jet reaches the surface, it creates a single-minded focus hypersonic shock wave which penetrates into the lithosphere at ∼10–100 km, expending their energy to evaporate, melting and heating of lithosphere rocks in accordance with the hydrodynamic theory of M. A. Lavrentiev [3].

Taking into account both mechanisms, we have shown [4] that all the main forms of relief surface of the terrestrial planets, such as craters, diatremes, lava flows, volcanoes, dome-shaped surface uplifts, as well as coronas and montes (on Venus) can be explained by falls of galactic comets at a combination of number factors. These factors are: 1) presence and density of planet's gaseous envelope, 2) lithosphere thickness, 3) composition and degree of heating rocks, 4) frequency of falls galactic comets.

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CONTINUAL THERMAL TREATMENT ON THE DETONATION DIAMOND CONTAINING MATERIAL

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Thermal treatment of diamond containing material obtained under detonation conditions in the interval of oxygen window 430 C to investigate changes in the structure of the this material particles was performed. The duration of the thermal treatment varied from 1 to 48 hours. Infrared and Raman experiments and dynamic light scattering of the treatment samples were carried out. The experiments did not confirm the existence of oxygen window. The structure of the particles of DCM is most likely to explain from the standpoint of the initial detonation density fluctuation influence on the particle formation.

ATOMIC NUMBER AND TEMPERATURE DEPENDENCE OF SHELL EFFECTS CONTRIBUTION IN PLASMA CHARACTERS

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The modern semiclassical method [1, 2] employs the TF statistical model and includes the shell and other physical effects by means of additive corrections. When using to describe the properties of plasma the method corresponds to the extreme matter states, i.e., to high temperatures. Purpose of the paper is to attract attention to some restraints, which one may be confronted with when using the approach at low temperatures.

The method [1, 2] substantially utilizes a smallness (in comparison with TF-term) and additivity of corrections. For high temperatures the smallness of shell correction and efficiency of its application were verified in the calculations of plasma ionicity and equation of state. However some additional assumptions were made to obtain the simple formula for the shell correction. The assumptions were confirmed at high temperatures, but they require proving or change when temperature decreasing.

The assumptions include: (1) the result depends only on a energy spectrum behavior near a point of chemical potential, (2) quadratic dependency assumption of the radial action on the orbital angular momentum, (3) neglect the orbital quantum number l discreteness. The last assumption means that a summation over l is substituted by integration.

It was shown in the paper of authors [3], that refusal of the approximation (3) substantially increases the accuracy of the semiclassical method when calculating ionization potentials of the free ions. However, it turned out that a plasma situation is much more complex and requires a more thorough study.

In the paper, we discuss the correctness of assumptions enumerated above when a plasma temperature decreasing and analyze results of their refusal by the example of calculating a number of single-particle states for a few elements with strongly differing atomic numbers.

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INCOMMENSURATE HOST-GUEST STRUCTURES IN COMPRESSED ELEMENTS: HUME–ROTHERY EFFECTS AS ORIGIN

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Discovery of the incommensurate structure in the element Ba under pressure 15 years ago [1] was followed by findings of a series of similar structures in other compressed elements (see reviews [2, 3] and references therein). Incommensurately modulated structures of host-guest (h-g) type consist of a tetragonal host structure and a guest structure in the form of chains embedded in the host atom channels so that the axial ratios of these subcells along c axis $\gamma = c_{host}/c_{guest}$ are not rational. We consider here two types of the h-g structures: (1) the host cell with 8 atoms; (2) the host cell with 16 atoms; for both types the guest cells contain 2 atoms adding to the h-g cell ($2 \times \gamma$) atoms.Examples are: $tI11^*$ in Bi, Sb, As and $tI19^*$ in Na, K, Rb, with the non-integer number of atoms in cell.

There is a close structural relationship of these h-g structures with the binary alloy phase Au_3Cd_5—$tI32$, space group $I4/mcm$. Cd atoms in position $16k$ form octagon—square nets same as alkali—host atoms in $tI19^*$. Au atoms in position $8h$ form square—triangle nets like Bi—host atoms in $tI11^*$. Atoms Cd in $4b$ and Au in $4a$ relate to guest atoms in chains with increased interatomic distances forming a guest subcell with the incommensurate c_{host}/c_{guest} ratio and reduced number of atoms in the structure to non-integer values.

The phase Au_3Cd_5—$tI32$ is related to the family of the Hume–Rothery phases that stabilized by Fermi sphere—Brillouin zone (FS-BZ) interactions where decrease in the electronic band structure energy occurs by the contact of the Fermi sphere and Brillouin planes [2]. This approach is used to analyze structure stability for the host-guest incommensurate structures by considering appropriate approximants. Following this consideration for alkali and alkali-earth elements is the necessity to assume the valence electrons band overlap with the upper core electrons and increase

of the valence electron counts to higher values under compression [4, 5].

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SEMICLASSICAL SIMULATION OF THERMODYNAMIC AND TRANSPORT PROPERTIES OF QUARK–GLUON PLASMA

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For quantum simulations of the thermodynamic and transport properties of the quark – gluon plasma (QGP) within a unified approach, we combine path integral andWigner (phase space) formulations of quantum mechanics [1.2]. The thermodynamic properties of a strongly coupled quark-gluon plasma (QGP) of the constituent quasiparticles are studied by color path-integral Monte-Carlo simulations (CPIMC). For simulations we have presented the QGP partition function in the form of a color path integral with a new relativistic measure, instead of a Gaussian that is used in Feynman andWiener path integrals. For integration over the color variable we have also developed procedure of sampling the color variables according to the group SU(3) Haar measure. It is shown that this method is able to reproduce the available quantum lattice chromodynamics (QCD) data. In the second part, the canonically averaged quantum operator time correlation functions and related kinetic coefficients are calculated according to the Kubo formulas. In this approach CPIMC is used not only for calculation thermodynamic functions but also to generate initial conditions (equilibrium spatial, momentum, spin, flavor and color quasiparticle configurations) for generating the color phase space trajectories being the solutions of the related dynamic differential equations. Correlation functions and kinetic coefficients are calculated as averages of Weyls symbols of dynamic operators along these trajectories. Using this approach we have calculated the diffusion coefficient and shear viscosity, which agree

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ON ANOMALOUS WAVE PROCESSES AT DIRECT AND REVERSE QUARK–HADRON PHASE TRANSITION

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The collective dynamic phenomena accompanying the collision of high energy heavy ions are suggested to be described approximately in the framework of ideal relativistic hydrodynamics. The anomalous behavior of shock and rarefaction waves (which is related to the shock wave stability problem) in the presence of phase transition may be manifested in energy and angular distributions of the reaction products. In the present work two aspects of the problem are considered. The first one is stimulated two-dimensional shock wave splitting with formation of the transverse shock waves. The possibility of the two-dimensional shock wave splitting was discussed in connection with the shock wave neutral stability condition [1, 2]. The principal difference between the case under consideration and one-dimensional shock wave splitting is the presence of transverse momentum which can affect the angular distribution of reaction products after collision. The solution of the initial value problem, which models two-dimensional shock-wave splitting in the presence of the perturbations, has shown damping of transverse waves and formation of plane shock wave of phase transition. The second problem is the sensitivity of temperature history in the expanding fireball to the flow geometry. The calculations have shown that in the cases of cylindrical and spherical flow symmetry as well as in the case of asymmetry, which models non-central collision, there is a time interval, in which the temperature of the expanding matter is concluded within the narrow temperature range $\delta T/T \approx 0.1$. This phenomenon can be explained by the formation composite rarefaction wave and relatively high value of the thermal capacity of the mixed phase, in accordance with the equation of state used in the calculations. It should be noted that the both discussed phenomena depend on the thermodynamic

properties of the matter. In the present work the simple equation of state based on the MIT-bag model is used [3].

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ANOMALOUS THERMODYNAMICS OF MATTER UNDERGOING ENTROPIC PHASE TRANSITION

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Subdivision of all 1st-order phase transitions (PT) onto two subclasses, i.e. enthalpic and entropic PT-s, were proposed in previous paper [1]. It was stressed that in contrast to ordinary enthalpic (e.g. Van-der-Waals-like) phase transitions the matter undergoing entropic phase transitions enters unavoidably in the region of anomalous thermodynamic properties where infinite number of cross second derivatives lose simultaneously their usual positiveness and became negative. Three most important are: Gruneizen coefficient, thermal expansion and thermal pressure coefficients. Negative sign of all these derivatives lead to numerous violation of standard order for most iso-lines, e.g. iso-T, iso-S, Hugoniots etc. These anomalies are under discussions. The region of discussed anomalous thermodynamics may coincide exactly with two-phase region in the case of *non-isostructural* entropic PT-s like melting and polymorphic PT-s. On the contrary, the anomalous thermodynamics region is *wider* than the two-phase region for isostructural entropic PT-s (e.g. PT of fluid-fluid type with critical end-point) and imply the latter inside the region of discussed anomalies. New remarkable thermodynamic object appears in this case – it is unknown yet boundary of domain with anomalous thermodynamics, where all discussed cross derivatives are *equal to zero* simultaneously. General properties and thermo- and hydrodynamic consequences of crossing this boundary by matter state parameters are under discussion. Several PT-s, obtained recently via approximate thermodynamic models or in frames of ab initio approaches, as well as those explored in recent

dynamic experiments, are classified onto enthalpic and entropic groups in accordance with criteria proposed in [1].

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THE SIMPLEST MODEL FOR NON-CONGRUENT FLUID–FLUID PHASE TRANSITION IN COULOMB SYSTEM

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The simplest model for non-congruent phase transition (NCPT) of gas-liquid type was developed in frames of modified model with no associations [1] of a binary ionic mixture (BIM) on a rigid ideal background (or non-ideal) electron gas/ BIM (#) /. The analytical approximation for equation of state (EoS) of Potekhin and Chabrier [2] of fully ionized electron-ionic plasma was used for description of the ion-ion correlations (Coulomb nonideality) in combination with "linear mixture" (LM) approximation. Phase equilibrium for the charged species was calculated according to the Gibbs-Guggenheim conditions [1].

The presently considered BIM (#) model allows to calculate full set of parameters for phase boundaries of non-congruent variant of phase equilibrium and to study all features for this NCPT realization in Coulomb system in comparison with the simpler (standard) forced-congruent evaporation mode. In particular, in BIM (#) there were reproduced two-dimensional remarkable ("banana-like") structure of two-phase region $P-T$ diagram and the characteristic nonmonotonic shape of caloric phase enthalpy-temperature diagram, similar to the non-congruent evaporation of reactive plasma products in high-temperature heating with the uranium-oxygen system [3]. The parameters of critical points (CP) line were calculated on the entire range of proportions of ions $0 < x < 1$, including two reference values, when CP coincides with a point of extreme temperature and extreme pressure, xT and xP. Finally, it is clearly demonstrated the low-temperature property of noncongruent gas-liquid transition - "distillation", which is weak in chemically reactive plasmas [4].

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AVERAGE ATOM APPROXIMATION IN NON-LTE LEVEL KINETICS

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Average atom approach assumes that an ion with average occupation numbers together with free electrons is contained in an electrically-neutral spherical cell. In this approximation the level kinetics equations can be written for mean occupation numbers with the rates calculated by using average atom wave functions. This model describes non-stationary ionization (recombination) processes with given radiation field. The possible extension of average atom model is connected with splitting average ion into set of ions representing a number of ion states.

The vice versa possible approach is based on reducing (averaging) the detailed atomic data base into extended average atom model. It gives radiative unresolved spectra atomic model, which may be used in-line in RHD calculations due to small computing time and acceptable accuracy. The calculation results of different approaches for some practical tasks are demonstrated.

HUGONIOT CALCULATION FOR CH AND CH_2 BASED ON HARTREE–FOCK–SLATER MODEL

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Calculated results are presented for Hugoniots of CH and CH_2 based on Hartree–Fock–Slater model with taking into account the band structure over a broad region of pressures and temperatures. The dependence of the

results obtained from the selected method of constructing the equations of state for the mixture. In particular, the technique of determining the self-consistent potentials for a mixture of simple substances proposed by Orlov [1] is applied. For the cell-based models of matter, this technique allows to make equal the chemical potentials those are calculated separately for each component of the mixture. The uniform free-electron density model, the Thomas–Fermi model and the Hartree–Fock–Slater model without taking into account the band structure are selected as other (more simple) quantum-statistical models for comparison. A comparison is done with results of other quantum-statistical approaches and available data from shock-wave experiments with CH and CH_2.

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THEORETICAL DESCRIPTION OF SHOCK HUGONIOTS OF METALS: PROBLEMS AND PERSPECTIVES

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In this work we consider different methods of calculation of shock Hugoniots of metals: analytical approaches, semiempirical equations of state, and first-principle calculations. The diffculties of theoretical interpretation of shock adiabats of metals is caused by a strong degeneration of electrons and high values of the coupling parameter along the Hugoniots. For the good quality of description both thermodynamic properties of electrons and ions should be taken into account by realistic models; for calculations at relatively low pressures accurate reproduction of the cold curve is necessary. We show that currently the density functional theory and quantum molecular dynamics methods provide good agreement with experimental data in wide range of parameters. The technical diffculties arise for very complicated structures in the crystalline state and at very high temperatures.

MELTING CURVES OF METALS WITH HEATED ELECTRONS BY AB INITIO CALCULATIONS

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In this work we reproduced melting curves for some metals up to 2 Mbar using *ab-initio* pseudopotential density functional theory calculations (VASP [1]). We applied the quasiharmonic approximation to determine thermodynamic properties and the Lindemann criterion [2] to build melting curves. We also investigated the influence of electron temperature on melting temperature at some isochors of metals under consideration in continuation of earlier studies [3, 4]. It turned out that the melting temperature increases with the rise of electron temperature at normal density and has non-monotonic behavior at higher densities.

Calculations were performed for aluminum, copper and gold. Results of our calculations of melting curves agreed excellently with available experimental data.

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THE NEW METHOD FOR CALCULATING THE SHELL CORRECTION TO THERMODYNAMIC FUNCTIONS IN THE SEMICLASSICAL APPROACH

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The problem of wide range equations of state remains unsolved nowdays. The most relevant models, such as DFT approaches, have computational difficulties and restrictions for the temperatures of the order 10 eV and for the low densities. However, a reliable equation of state for the warm dense matter is possible to obtain with simplified approaches such as semiclassical average atom model. The semiclassical approach [1] for the calculation of thermodynamic functions of electrons has been devel-

oped to extend the region of validity [2] of the Thomas-Fermi model at finite temperatures. The calculation of the shell correction here is of high importance because it provides thermodynamic functions with the information about bound states of electrons which is necessary for the step-wise inoization [3].

The method for calculating the shell correction, which was firstly proposed by G. V. Shpatakovskaya, has been essentially modified by the authors. Multiplicity of assumptions used earlier was too difficult to check numerically. Modern numerical algorithms applied at powerful computers allowed us to eliminate these disadvantages and enhance the precision.

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EQUATIONS OF STATE OF NOVEL MATERIALS DISCOVERED FROM EXTREME CONDITIONS

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The pressure-volume-temperature equations of state of a number of newly synthesized compounds under extreme pressure-temperature conditions (semiconducting magnesium carbides and boron suboxides, metallic sodium silicides, silicon allotrope with quasi-direct bandgap, allotropes of boron, etc.) will be presented.

EQUATION OF STATE OF METALLIC PLASMA

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Equation of state of metallic plasma produced under conditions of electric explosion is reported. Problem of correct theoretical description of these data is formulated and discussed. Regions of the phase diagram of metal accessed with the use of different experimental techniques of explosion metallic wires and foils are analyzed and compared with possibilities of shock-wave methods.

STUDY OF NEAR-CRITICAL STATES OF LIQUID–VAPOR PHASE TRANSITION OF MAGNESIUM

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Study of thermodynamic parameters of magnesium in the near-critical point region of the liquid-vapor phase transition and in the region of metal-nonmetal transition was carried out. Measurements of the electrical resistance of magnesium after shock compression and expansion into gas (helium) environment in the process of isobaric heating was carried out. Heating of the magnesium surface by heat transfer with hot helium was performed. The registered electrical resistance of expanded magnesium was about 10^4-10^5 times lower than the electrical resistance of the magnesium under normal condition at the density less than the density of the critical point. Thus metal-nonmetal transition was found in magnesium.

INFLUENCE OF SOLID-STATE CHARACTERISTICS ON CRITICAL PARAMETERS OF VAPOR–LIQUID PHASE TRANSITION

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In the review [1] a number of observations are made about possible influence of solid-state characteristics under normal conditions on properties of a liquid phase, and also "supercritical fluid". The later one are determined as a gaseous phase of substance on near critical density, temperatures and pressure. In a series of our works [2, 3] devoted to vapor-liquid (dielectric-metal) phase transition in metal vapors, atomic hydrogen and excitons the similar idea of cohesive binding energy is used. This energy obtained actually for the ordered (condensed) system of atoms allowed us to calculate critical parameters of vapor-liquid transition using a gas-liquid equation of state. Thereby existence of solid-state and gas parameters binding is directly shown. Cohesive energy arises in the dense vapors of metals due to appearance of a conducting band and conduction electrons. In this study, using the universal ratio for binding energy [4] the vapor-liquid phase transition in inert gases and mercury is considered. Cohesive energy in this case has absolutely other nature, than in metals. It's rather classical. For these substances the cohesive binding energy is

recovered by us on the basis of the solid-state properties found in literature and the universal ratio for binding energy (UBER). For calculation on the basis of UBER we used: evaporation heat, solid-state density and elastic modulus. Critical parameters of phase transition from liquid to a gaseous state are calculated using the free energy of an atomic fluid [2, 3]. The obtained results are compared to the experimental data and data of numerical calculations. The obtained unexpectedly good agreement with experiment can serve as direct confirmation of the ideas stated in [1] about relation of solid-state parameters with properties of "a supercritical fluid" and with critical point parameters.

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THERMODYNAMICAL DESCRIPTION OF THE LIQUID METALS AT PULSED ENERGY FLOWS IMPACT

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The work is devoted to the problem of the description of the liquid metals at pulsed energy flows impact. According to J. I. Frenkel, to suppose, that melting occurs as a result of a lattice stability loss due to the avalanche-like growth of the Frenkel pairs ("vacancy-interstitial atom") in the vicinity of the melting temperature (T_L). The molten metal at the melting curve can be represented as a mixture of clusters and vapor, partly filling intercluster (free) volume. The symmetry defining clusters oscillatory spectrum differs from the crystal symmetry at the melting curve and can be described within the Debye model, or the Einstein model, or even as a superposition of spectra of these models. Free energy of the melt equals to the sum of clusters free energies, which in a first approximation equals to the free energy of solid state with the formed lattice defects, ideal gas and electron gas with variable number of particles.

A new wide-range two-phase equation of state of metals is proposed. Free parametrs of Gibbs potential for liquid Na and Cu at $P = 10^5$ Pa are estimate. Melting curves of metals are defined within both one-phase approximation using Lindemann criterion, and two-phase-approximation.

Volume and entropy discontinuities are calculated as a function of pressure at melting curve for Na and Cu. We also compared all the simulations results to the available experimental data for the metals.

The work is carried out under the partial financial support of the RFBR (project No. 13-08-00266-a, project No. 14-08-31024-mol) and UB RAS within the UB RAS fundamental research program "Matter at high energy densities" (project No. 12-P-1005, state registration No. 01201266835).

CALCULATION OF ELASTIC MODULES BEHIND STRONG SHOCK WAVE

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In the paper the approach for calculation of mechanical characteristics of materials behind strong shock waves is realized in the frame of uniform system of the few-parametric equation of state [1]. For the considered materials a comprehensive comparison of theoretical computational results with available at high energy density experimental data is carried out and good agreement of the results is obtained.

The expression obtained for the Grueneisen coefficient allows one to find the equation for the zero isotherm and to analytically calculate the value for the "cold" components of pressure and internal energy and, hence, the thermodynamic expression of state for the solid phase with the thermal oscillations of the crystalline lattice are described by the Debye approximation.

Two-dimensional problems of the impact of model reactor blocks of a nuclear powerplant on the Earth surface (sandstone, granite, water) were solved numerically on the basis of the elastoplastic model and with the use of the constructed equation of state. The reactor impact on the Earth's surface at speeds more than 400 m/s leads to the reactor depressurization and consequently to possible radioactive contamination of the reactor impact point. The deformation and impact modeling details are described in [2]. The destruction problem of a nuclear powerplant of space power installation at space debris impact in orbit (impact velocity of 12 km/s) was solved on the basis of the obtained equation of state in the two-dimensional formulation. The results show that high-velocity debris impacts lead to catastrophic failure of the reactor.

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GRÜNEISEN COEFFICIENT VOLUME RELATION OF THE TATB MOLECULAR CRYSTAL

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This work described the analysis expressions of Grüneisen coefficient volume relation $\gamma(v)$ from the viewpoint of the construction of the molecular crystalline material state equation. Regression analysis results was compared to the available experimental data for explosive TATB that was gained in the static shock-wave experiments. All concerned expressions for $\gamma(v)$ in normal cases γ_0 and in the range of low pressures predict Grüneisen coefficient value with fine accuracy, but in the limit of infinite compression this experiments can not give correct values. One of the causes of this effect is low pressures condition for the experiment. In the course of analysis it was proposed Grüneisen coefficient volume relation expression for construction of triamino-trinitrobenzene state equation.

THERMAL COMPONENT IN THE EQUATION OF STATE FOR TRIAMINO TRINITROBENZENE

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Considerable success has been achieved in studying the P-V-T properties of high-molecular organic compounds which also include explosives (HE). But theoretical determination of relationships characterizing behavior of solid explosives runs into difficulties as they belong to molecular crystals and molecules constituting a crystal have great many internal degrees of freedom. The equation of state was constructed based on the definition of the Helmholtz free energy F (V,T) related, in the most simple way, to the

structural model of the matter in the assumption of pressure and energy represented as thermal and potential (elastic) components. The potential component depends on the type of a solid body and on the attractive and repulsive forces existing in a particular molecular crystal. The thermal component is determined by the oscillatory motion of molecules. Given that normal oscillation frequencies inside a molecule are one order of magnitude higher than those of normal oscillations of a molecule as a whole, two characteristic temperatures can be derived and the low-, and high-frequency components can be distinguished in the oscillatory component of the free energy. The Debye approach used to describe the low-frequency component of the free energy and the Einstein approach used to describe high-frequency component thereof helped to obtain a semi-empirical equation of state for the molecular crystal. The proposed equation of state is used to describe thermodynamic properties of triamino trinitrobenzene

ON SOME PROPERTIES OF FRACTAL OSCILLATOR EQUATION

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The development of mathematical physics of fractals has attracted considerable interest in the physical and biological systems of fractal organization, oscillates about the position of stable equilibrium, - to fractal oscillators and their equations [1],[2].

Equation

$$\frac{1}{\Gamma(2-\alpha)}\int\limits_0^t \frac{u''(\tau)d\tau}{(t-\tau)^{\alpha-1}} + \omega^\alpha u(t) = 0, \;\; 1 < \alpha = \text{const} < 2, \; \omega = \text{const} > 0, \tag{1}$$

F. Mainardi [3] called Fractional Oscillating Equation.

Let

$$D_{0t}^\alpha u(\tau) = \sum_{k=0}^{n-1} \frac{u^{(k)}(0)}{\Gamma(1+k-\alpha)} t^{k-\alpha} + \partial_{0t}^\alpha u(\tau), \;\; \alpha \in]n-1, n], \; n = 1, 2, ...,$$

where $\Gamma(z)$ – Euler gamma function; $\partial_{0t}^\alpha u(\tau) = D_{0t}^{\alpha-n} u^{(n)}(\tau)$.

Equation (1) is equivalent to the following equation [1, p.181]

$$u''(t) + \omega^\alpha D_{0t}^\varepsilon u(\tau) = 0, \;\; 0 < t < T, \; \varepsilon = 2 - \alpha. \tag{2}$$

The report will examine the qualitative properties of solutions of equation (2), and give their application to a variety of physical processes, in particular, to the Boussinesq equation with a discontinuous time diffusion coefficient [4].

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SMALL NUMBER PARAMETERS EQUATION OF STATE WITH A FRACTIONAL DERIVATIVE

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In this paper, the operator of fractional integro-differentiation Riemann - Liouville used to construct the equation of state of a solid with fractal structure. According to the definition, the pressure through the free energy can be expressed by the following formula

$$p = -\left(\frac{\partial F}{\partial V}\right)_T = -\frac{1}{V_0}\left(\frac{\partial F}{\partial x}\right)_T, \tag{1}$$

where F - free energy, V_0 - volume occupied by one particle, $x = V/V_0$ dimensionless volume. In the analogue Newton-Leibniz formula in the fractional calculus [1], and given the fact that the free energy F is continuously dependent on the volume, we obtain ratio

$$\frac{dF(x)}{dx} = D^{\alpha}_{0x} D^{1-\alpha}_{0x} F(x), \quad 0 < \alpha < 1, \tag{2}$$

$$D^{\alpha}_{0x} F = \frac{1}{\Gamma(1 + [\alpha] - \alpha)} \frac{d^{[\alpha]+1}}{dx^{[\alpha]+1}} \int\limits_0^x \frac{F(t)dt}{(x-t)^{\alpha-[\alpha]}}, \tag{3}$$

where D_{0x}^{α} fractional differentiation operator in the sense of Riemann-Liouville order α [1,c.9]: The paper presents two different equations of state:

$$p = \frac{1}{V_0} \sum_{n=0}^{N} a_n \frac{x^{n-a}}{\Gamma(n-\alpha+1)}. \tag{4}$$

$$p = \frac{c}{V_0} x^{-\alpha}. \tag{5}$$

In this paper the equation of state of a solid using a fractional derivative of Riemann-Liouville and the expression for the free energy and the bulk modulus. The resulting equation of state is supposed to be used to predict the thermodynamic properties of substances with a fractal structure.

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THREE BODY POTENTIAL FOR EOS OBTAINED IN THE FRAME OF MOLECULAR DYNAMICS METHOD

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Thermodynamic parameters calculations for inertial gases based on binary central potentials using a program for molecular dynamic simulation LAMMPS provide for critical temperatures an accuracy of 6% for xenon and only 17% for krypton [1]. For three body interaction approximation the pressure P versus one particle volume v is expressed in the form

$$P = \frac{k_B T}{v} + \frac{B}{v^2} + \frac{C}{v^3}, \tag{1}$$

$$B = -\frac{2\pi}{3} \int_0^{\infty} F_2(r) \frac{d\Phi^{(2)}}{dr} r^3 dr \ , \tag{2}$$

where F_2 and $\Phi^{(2)}$ are two particle distribution function and a central potential. Coefficient C is expressed through tertiary distribution functions $F_3(\mathbf{r_1}, \mathbf{r_2}, \mathbf{r_3})$ and three body interaction potential $\Phi_{ijk}^{(3)}$, which is defined by the three particle energy E_{ijk} [2]

$$\Phi_{ijk}^{(3)} = E_{ijk} - \Phi_{ij}^{(2)} - \Phi_{ik}^{(2)} - \Phi_{jk}^{(2)} - 3E_0. \tag{3}$$

$\Phi^{(3)}_{ijk}$ depends on 6 algebraically independent polynomials that are invariant under transformations of the group $O(3)\times S_3$ composed of the radius vector of the particle i, j and k [3]. We analyze the dependence of $\Phi^{(3)}_{ijk}$ on two invariants

$$I_1 = \mathbf{r}_{12}^2 + \mathbf{r}_{23}^2 + \mathbf{r}_{13}^2, \tag{4}$$

$$I_2 = \mathbf{r}_{12}\mathbf{r}_{23} + \mathbf{r}_{23}\mathbf{r}_{31} + \mathbf{r}_{31}\mathbf{r}_{12}. \tag{5}$$

Parameters of three-particle potential have been chosen using three-particle energy E_{ijk} calculated in the frame of density functional method.

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TWO-TEMPERATURE EQUATIONS OF STATE AND LATTICE STABILITY OF COPPER AND GOLD

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In this work the model of thermodynamic and transport properties of copper and gold at electron-ion non-equilibrium is presented. Accepted in the model ranges of electron temperature and pressure are enough to describe the experimentally achievable states [1, 2]. The changes in electron spectra due to electron heating and compression or expansion are taken into account with the help of two-parabolical model developed in [3]. In the cited work thermal conductivity and electron-ion coupling was considered as dependencies from electron and ion temperatures. Now the dependence from density for these coefficients is taken into account. To include exchange-correlation effects on electron-electron collisions we have found out how this effect can be included in electron screening. Also we have renewed our approach for heat conductivity calculation to include thermoelectric phenomena which are significant at high electron temperatures. The lattice stability [4] of solid copper and gold at electron-ion non-equilibrium is investigated; particularly, the effect of electron heating on sound velocities in metals called above. The two-temperature hydrodynamics simulation of film expansion was provided with the use of the

model presented here. This work was supported by RFBR (grant No 13-02-01078).

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THERMODYNAMIC, TRANSPORT AND OPTICAL PROPERTIES OF PLASTICS BY THE AB INITIO CALCULATION

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The plastics are widely used in high energy density physics. The usage of plastics for the contrast improvement of intense laser pulses [1] is an example of such a fruitful application.

The information on the matter properties is necessary to perform numerical simulation of the experiment. In this work we obtain thermodynamic, transport and optical properties of plastics by the *ab initio* calculation. The calculation is based on the quantum molecular dynamics, density functional theory and the Kubo-Greenwood formula. The detailed description of method, choice of technical parameters and comparison with other works is available for aluminum in paper [2].

The plastics of the effective composition CH_2 were investigated at $\rho = 0.954$ g/cm^3 and temperatures 5 kK $\leq T \leq$ 100 kK.

The pressure without kinetic contribution of ions $p - p_i^{\text{kin}}$ is almost constant at 5 kK $\leq T \leq$ 10 kK and grows at 10 kK $\leq T \leq$ 100 kK, total pressure p grows monotonically at 5 kK $\leq T \leq$ 100 kK. Thermal conductivity $C_v = dE/dT$ decreases at 5 kK $\leq T \leq$ 15 kK and increases at 15 kK $\leq T \leq$ 100 kK.

The dynamic electrical conductivity $\sigma_1(\omega)$ at 5 kK has non-Drude shape with peak at 10 eV; the curves are smoother at higher T.

Static electrical conductivity $\sigma_{1_{\text{DC}}}$ demonstrates step-like behavior—

it grows rapidly at 5 kK $\leq T \leq$ 10 kK and is almost constant at 20 kK $\leq T \leq$ 60 kK. Thermal conductivity grows monotonically at 5 kK $\leq T \leq$ 100 kK.

The density of the electron states (DOS) was investigated to explain rapid growth of $\sigma_{1_{\mathrm{DC}}}$ at 5 kK $\leq T \leq$ 10 kK. At 5 kK the chemical potential μ corresponds to the dip at the DOS curve, the values of $\sigma_{1_{\mathrm{DC}}}$ are low. At 10 kK the DOS at μ is larger than at 5 kK, thus $\sigma_{1_{\mathrm{DC}}}$ at 10 kK is also larger than at 5 kK.

This work was supported by the Ministry of Education and Science of the Russian Federation, grant No. 3.522.2014/K.

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PRESSURE IN ELECTRONICALLY EXCITED WARM DENSE METALS

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Irradiation of solids with ultrashort laser pulses opened an exciting field of research. New emerging physics is connected with formation of warm dense matter (WDM) at the initial transient state of material evolution after energy deposition into electron subsystem. WDM in such ultrafast phenomena is a non-equilibrium state that makes it very challenging for theory, modelling and simulation. Usually WDM can be described as a two-temperature (2T) system when electron and ion subsystems can be considered in quasi-equilibrium at $T_e > T_i$.

Physics of WDM is not a subject of pure fundamental interest. One of the major phenomena where WDM properties are crucially important in modelling and simulation is laser ablation. Laser ablation is a multiscale phenomenon. Subpicosecond laser excitation transforms material under normal conditions into 2T-WDM in the isochoric way. Relaxation takes about tens of picoseconds before T_i and T_e become equal. This relaxation stage governs the details of ablation mechanism and is the focus of the on-going modelling effort. It can be described at the continuum level. However atomistic modelling gives the possibility to capture a richer spectrum of structural transitions and nucleation effects.

In this work we discuss two connected questions. On examples of aluminum and gold using the finite temperature Kohn-Sham density functional theory (FT KS DFT) we are making an attempt to analyze the electronic contribution to the total pressure in 2T-WDM metals [1]. Another question is the separation of electrons into bound and free that is a general problem for non-ideal plasma physics.

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RECENT ADVANCES IN LASER-PULSE MELTING OF GRAPHITE AT HIGH PRESSURE

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Melting temperature of graphite and nature of liquid carbon remains a subject of permanent discussions in the literature for many decades. The main reason of this inconsistency is the extremely high melting temperature of graphite making it the most refractory material. Moreover, melting of graphite is possible only at pressures higher than ca. 100 bar (this latter is stated by most of researchers). The present study deals with a further improvement of the laser-heating technique first used in [1] with the aim to reach a higher reproducibility of the results, to improve and to broaden means of optical measurements and to better control the process of cooling and freezing of liquid carbon.

Very high reproducibility of the heating thermograms is achieved, which allowed one to make more precise evaluation of the knee point at the ascending flank of the thermogram first reported and interpreted in [1]. The frozen liquid carbon and the adjacent area are studied using the SEM microscopy. The peculiarities of melting of graphite and freezing of liquid carbon are discussed. Distinctive feature of the present study is the use of high speed video observation in reflected light of formation of liquid carbon, which has been successfully performed in spite of extremely intensive thermal radiation of condensed carbon at temperatures at the vicinity of 5000 K. New data on estimation of liquid carbon density along with the peculiarities of vaporization of liquid carbon and condensation of carbon vapor in the pressure range up to 5 kbar are presented.

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ON THE KINETICS OF GRAPHITE MELTING: A MOLECULAR MODELING APPROACH

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Unique thermophysical properties of graphite result in its important role in science and engineering. However, the experimental data on graphite melting temperature (T_m) still remain controversial despite the long history of investigation. The experimental results of several works cover the wide span from 3800 to 5000 K that is an essentially larger uncertainty than the errors of individual experiments. In this work we deploy the molecular dynamics (MD) method and expand our previous study of the kinetics of graphite melting [1]. We consider the melting front propagation rate, the aspects of defect formation, single graphene layer melting and the rates of spontaneous liquid nuclei formation. On the basis of an accurate interatomic potential for carbon (AIREBO) we determine by thermodynamics integration method the value of $T_m \approx 3650$ K. We discuss the dependence of this value on the interatomic interaction model deployed.

Our MD calculations show an unexpectedly weak kinetics of the melting front propagation in graphite that is several orders slower than that in metals. We demonstrate that at sufficiently high heating rates (higher than $10^5 - 10^6$ K/s) the temperatures 500-1000 K above the graphite melting temperature can be reached before the crystal decay. It allows us to propose an explanation for the long-standing problem of the discrepancy in the experimental data on the graphite melting temperature making a hypothesis that experimentally detected temperatures could be systematically biased due to graphite superheating and this bias depends on the heating rate [2].

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PHASE TRANSITION IN THE FILM OF LIQUID CARBON UNDER INTENSIVE HEAT TRANSFER WITH THE COLD DIAMOND SUBSTRATE: MOLECULAR-DYNAMIC SIMULATION

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Liquid carbon ($T = 6600$ K) quenching on the cold diamond substrate at $T = 300$ K in conditions close to the experimental laser melting of dispersed graphite on a substrate of natural diamond is investigated using molecular dynamics (MD) simulations. Quenching was carried out for two types of boundary conditions on the side opposite to the diamond substrate. The simulations confirmed the experimental result of the formation of amorphous carbon under such conditions. The calculations show that the destruction of diamond didn't take place because of its very high thermal conductivity. The estimation of the cooling rate of liquid carbon was done. The result is 10^{15} K/s, that is agrees with the literature data, where it is shown that such a high cooling rate is typical for amorphous carbon formation in industrial processes, and for "production" of amorphous carbon in atomistic modeling. Temperature profiles in different layers of liquid carbon were restored to reproduce the detailed picture of the quenching process. We also performed a thorough topological analysis of amorphous carbon obtained in MD simulation. In the present work, we evaluate the radial distributional function (RDF), the average distribution of carbon atoms depends on the covalent bond type in carbon: sp^1-sp^2-sp^3, the distribution of the average bond length between two nearest carbon atoms, the distribution of the azimuthal angles formed by the three nearest carbon atoms C-C-C. This analysis confirmed that the amorphous carbon obtained by quenching in MD simulations had a graphite-like structure (86.5% of the atoms were linked by the covalent sp^2 bond).

This work was supported by the Russian Foundation for Basic Research (Grant 13-08-01098a).

MOLECULAR DYNAMICS SIMULATION OF MELTING AND SUPERIONIC TRANSITION IN VARIOUS STRUCTURES: UO_2, UN_2, TiH_2

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It is considered that structures of fluorite type (type CaF_2) can have superionic transition at temperatures comparable to melting temperatures. Superionic transition is a process when atoms of one type leave their positions and begin to move in field of second type atoms, while the last preserve crystal state. There are some models of mechanism of this transition. Superionic transition can be explained by high probability of defects formation in one of sublattices. One of characteristics of this process is high growth of capacity (both electric and heat). At present time it is discussed to which type of transitions (first or second order) this phenomenon belongs to.

In this work, various systems had been studied using molecular dynamics simulation (MD). In particular, superionic transition in UO_2 was investigated. The dependency of heat capacity on temperature had been studied near superionic transition point. A comparison with theoretical models of phase transitions was done. The dependency of defects concentration on temperature was obtained as result of the simulation. An activation energy of the process was calculated.

In addition, superionic transition and melting were studied in UN_2 and TiH_2. UN_2 did not show superionic transition explicitly. However, spinodal decomposition from solid to liquid state has features of superionic transition.

THE INVESTIGATION OF PHASE TRANSITIONS IN URANIUM MONONITRIDE WITH USING OF THE MOLECULAR DYNAMICS SIMULATION

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Uranium nitride (UN) is the perspective fuel which ones going to use in forth generation nuclear reactors. It has plenty of advantages over uranium dioxide for instance high temperature of melting point, high conductivity or high density. Unfortunately physical properties of this substance was

not studied well. One of the important tasks of radiation material science is the study of phase diagram in wide range of pressure and temperature.

In this work using the molecular dynamics with novel interatomic potential we have studied phase transitions in UN. The large part of the work is the study of the phase transition from cubic structure to rhombohedral structure at high pressure. Based on the performed simulation, the pressure of the transition is about 32 GPa at low temperatures. This value well agrees with available experimental data [1]. It is shown the type of rhombohedral structure depends on pressure. In addition the melting process of UN was simulated at wide range of pressure. Results of the work is compared to other theoretical models [2, 3].

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THERMODYNAMICS AND DIFFUSIVITY OF POINT DEFECTS IN UN: ATOMISTIC SIMULATIONS

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The present work is devoted to description of phase composition and concentration of point defects in the UN nuclear fuel, which is useful for analysis of the dissociation and sintering of the nitride fuel. The data on concentrations and diffusion coefficients of the defects are important for microscopic description of the release of fission products during burn-out of the nuclear fuel.

The model for description of concentrations and diffusion coefficients for point defects depending on deviation from the UN stoichiometric composition is proposed basing on the molecular dynamics simulations and calculations within electron density functional theory. Quantum mechanical static calculations are used for fitting of the parameters of the interaction potential (in the form of the embedded atom model with angular-dependent components) and evaluation of the defects formation and migration energies. Molecular dynamics simulations are aimed to analyze what migration mechanisms are activated at finite temperatures and to calculate diffusion coefficients of point defects.

It is shown that U-antisite defects (U in a regular site of N) play an

important role in the U-rich UN_{1-x}. Moreover, during a migration of U-interstitial U atom is able to knock-out N with the formation of U-antisite and N-interstitial. This effect results in a strong dependence of the diffusivity of U-interstitials on the concentration of defects in the N sublattice, which is important for rates of the diffusion-controlled reactions in the nitride nuclear fuel. The other peculiarity of UN in comparison with UO_2 is the large athermal concentration of U-vacancies in the N-rich UN_{1+x} due to a close formation energies of N Frenkel pairs and Shottky defects (pair of U and N vacancies). The predictions of the model are compared with the available experimental data on the stability range of the mononitride phase and self-diffusion coefficients of U and N.

DEVELOPMENT OF THE ATOMISTIC MODEL FOR ZIRCONIUM

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The alloys based on Zr are of great interest because of their application in nuclear reactor environments (as a cladding material). Nevertheless, possible formation of metastable phases in the Zr-based alloys can cause embrittlement of the cladding. Peculiarities of these phase transitions are not clear and require additional study.

In the present work a new interatomic potential for Zr is presented. The potential is set in a form of "Angular-dependent potential". It is based on *ab initio* data computed for some reference structures of hcp, bcc and liquid Zr. The potential obtained is used for molecular dynamics simulation of Zr properties. The results of simulations are discussed and compared to the other theoretical and experimental data for Zr.

MOLECULAR DYNAMIC STUDY OF METAL NUCLEAR FUEL FEATURES

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Uranium has received a lot of attention for its unique nuclear properties and its various applications in nuclear industry. In order to improve mechanical properties and corrosion resistance of uranium at room temperature while maintaining the high density, uranium is frequently alloyed with other elemental metals. Mo exhibits a high solubility in γ-U. Compared with other high density uranium alloys and compounds, the low-enriched uranium alloys with 6-12 wt.% of Mo have attracted a great deal of attention and are recognized as the most prominent candidates for advanced research and test reactors, because they have a relatively larger γ phase region and present more stable irradiation performance. Mo is a strong γ-stabilizer which provides stable swelling behavior in U-Pu-Mo fuels, has high thermal conductivity, low thermal expansion, and high melting points.

The method of atomistic simulations was used to study the structure of the quasi-equilibrium tetragonal phase U-Mo, formed during crystallization of the melt. The lattice constants of the uranium-molybdenum alloy were obtained for different concentrations of molybdenum. Results of calculations are in good agreement with experimental data and confirm the anisotropy of the lattice at low molybdenum concentrations. Temperature of the transition from anisotropic tetragonal phase to a body-centered cubic phase was calculated for different concentrations of molybdenum. It was found that the anisotropy is a consequence of the local arrangement of uranium atoms in the U-Mo alloy structure. It is shown that the anisotropy disappears with increase of molybdenum concentration not due to changes in the uranium atoms arrangement. It disappears because the number of molybdenum atoms - "stabilization centers of isotropy" increases. Also in the work dependence of the enthalpy of mixing for uranium-molybdenum alloy on molybdenum concentration was calculated. It is shown that anomalous enthalpy of mixing - molybdenum concentration dependence, known from the experiments, can be obtained only when the atomic structure of the alloy is taking into account. Properties of U-Mo alloy were compared with U-Zr alloy properties.

MULTI-SCALE MODEL OF THE DYNAMIC FRACTURE OF MOLTEN AND SOLID METALS

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A multi-scale model of the tensile fracture of metal melts is developed on the basis of combination of the molecular dynamics (MD) simulations with the continuous description of kinetics and dynamics of voids; the model considerably extends the time and spatial scales of MD. In the case of melts, the continuous model is the most simple and consists of the equation for voids nucleation due to the thermal fluctuations and the well-known Rayleigh-Plesset equation for their subsequent growth. Using of the literature data on the surface tension and viscosity of melts allows us to get a correspondence between the continuous description and MD. With the use of the model, we calculated the strength of the uniform melts of Al, Cu, Fe and Pb within a wide range of strain rates (from 10^3–10^4 to 10^9–10^{11} s^{-1}) and temperatures (from melting temperature to 70–80% of critical temperature). For solids, we propose a dislocation-based model of the void growth. The model is verified, and the parameters of the model are determined on the basis of MD simulations. Basing on the MD simulations, we also investigate the nucleation rates of voids in the uniform monocrystalline metals and metal melts, as well as dynamics of pre-existing pores. The results of MD simulation correspond with our continuous modeling. The nucleation rate of voids in the solid metals is described by the same law as in the case of the metal melt. Calculations show that the tensile strength of homogeneous melt decreases slowly with the strain rate decrease. As a result, within the range of the strain rates of 10^6–10^8 s^{-1}, a homogeneous nucleation mode can be realized, in which the dynamic strength of melt can be comparable or even higher than the strength of solid metal at room temperature. We proposed a schema of experiment for measurement of the tensile strength of uniform metal melts (fracture in the mode of homogeneous nucleation). The required conditions can be achieved at the irradiation of a metal plate by a high-current electron beam with the energy of electrons of about 1 MeV.

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TWO LEVEL DESCRIPTION OF DISLOCATION STIMULATED GROWTH OF NANOVOIDS UNDER HIGH RATE TENSION OF ALUMINUM

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With the help of molecular dynamic simulations [1] the mechanism of nanovoid growth in aluminum under high rate tension was studied. We interpret the growth of nanovoids as the result of plastic deformation in zone close to void and the corresponding atom rearrangement on void surface. The dependencies of critical negative pressure in systems of various atom number and void diameter at various temperatures was researched. It was shown, that critical pressure depends both on void diameter and simulated area size. The increase of temperature leads to linear decrease of system tensile strength.

The continual model connecting void growth rate with dislocation processes occurring around void is offered. The generation of dislocations near void surface is described with the Arrhenius type relation, the parameters of this formula (energy of dislocation nucleation and activation volume) are fitted by comparison with molecular dynamic data. When material deforms at rate of 0.01-0.1 1/ns, the initial dislocation density is enough for effective void growth, for grater deformation rates the dislocations nucleate near void surface.

The work is supported by the grant from the Russian Science Foundation, project 14-11-00538.

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ATOMISTIC SIMULATION OF NUCLEATION IN METASTABLE LIQUID METALS UNDER TENSION

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Under the action of high energy density fluxes the melting of metal is probable and fracture starts in a liquid phase. However the models for description of fracture kinetics in such a conditions, reached just for a short time, are hard to verify experimentally. The subject of this work is

the study of metastable liquid metals under tension by means of atomistic simulations. In this work nucleation rate in liquid Fe is calculated and is compared with data on nucleation rate in liquid metals with various surface tension. The results of this simulation could be applied to understand of nucleation in liquids under high strain-rate tension. Nucleation rate in liquid iron was calculated from molecular dynamics simulations basing on the average lifetime of the metastable state until formation and growth of cavity. The data on nucleation rate thus obtained was approximated in two ways: within classic nucleation theory - CNT [1] and within CNT with Tolman correction for the surface tension. Both approximations were compared. Tolman correction takes in consideration the dependence between surface energy and size of the bubble, or cavity in our case. Direct application of CNT to the approximation of the nucleation rates (with the surface tension available from the independent calculations) leads to an overestimation of the kinetic prefactor, which contradicts to the basics of CNT. Tolman length was estimated independently from the simulations and compared with Tolman length given by fitting with CNT with Tolman correction. It was ascertained that nucleation is well-described by CNT with Tolman correction in both Al and Fe with close values of the Tolman length. Also the results obtained by CNT were compared with dynamic calculations.

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SHAPE MEMORY PHENOMENA AND X-RAY DIFFRACTION STUDIES ON COPPER-BASED SHAPE MEMORY ALLOYS

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Shape memory effect is an unusual property exhibited by certain alloy systems, shape memory alloys. Shape memory effect is based on a solid state phase transition, martensitic transformation, which occurs on cooling in the material. Martensitic transformation has displacive character, and the changes in the crystal structure of the material at the nano-level rather than micro-level govern the transformation. The physical nature of shape memory concept is shape change in bulk level and lattice changes in crystallographic level. Martensitic transformations occur as martensite variants the lattice invariant shears on {110}-type planes of austen-

ite matrix, which is basal plane of martensite. The martensite variants are formed without causing any macroscopic deformation as lattice twins in self-accommodating manner. Deformation of shape memory alloys in martensitic state proceeds through a martensite variant reorientation or detwinning of twins. Copper based alloys exhibit this property in β-phase field. The high temperature bcc-structure of these alloys martensitically undergo to non-conventional layered structures on cooling from high temperature austenite phase following two ordered reactions. Lattice invariant shears are not uniform, and these shears cause the formation of the unusual layered structures which consist of an array of close-packed planes with complicated stacking sequences called as 3R, 9R or 18R martensites depending on the stacking sequences on the close-packed planes of the ordered lattice. The parent phase has high symmetry, and product phase has low symmetry; the unit cell and the periodicity are completed through 18 layers in z-direction in case of 18R structure.

In the present contribution, x-ray diffraction studies were carried out on two copper based ternary alloys; Cu–26.1%Zn–4%Al (in weight) and Cu–11%Al–6%Mn (in weight). X-ray diffraction patterns exhibits superlattice reflections in the quenched case. The alloy specimens were aged at room temperature, and a series of x-ray diffractograms have been taken during the ageing duration. These diffractograms reveal that peak locations and peak intensities change with ageing duration. This result refers to the rearrangements of atoms in diffusive manner. In conclusion, the changes in the location and intensities of diffraction peaks reveal the rearrangements of the atom in displacive manner; and this result provides us information on the degree of ordering in the martensitic state of the material.

SPIN CROSSOVER AND MOTT–HUBBARD TRANSITION UNDER HIGH PRESSURE AND HIGH TEMPERATURE IN THE LOW MANTLE OF THE EARTH

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A review of unusual magnetic, electronic and structural properties of Mott insulators induced by spin crossover is given. Spin crossover from the high spin (HS) to the low spin (LS) state often is induced by high pressure. It is the quantum phase transition at $P = P_C$ and zero temperature $T = 0$. At finite T crossover from HS to LS is smooth. Examples of spin crossover in $3d$-metal oxides are given. Spin crossover effect on

effective Hubbard U parameter is not universal and depends on the ionic configuration, U_{eff} degreasing for d^5-ion and increasing for d^6-ion. Thus spin crossover can decrease or increase the critical pressure determined by standard bandwidth control mechanism of the Mott-Hubbard transition.

High pressure induced spin crossover in ferropericlase $Mg_{1-x}Fe_xO$ is discussed. The low temperature P, T phase diagram has the quantum critical point $P = P_C = 55$ GPa at $T = 0$. It was found by the synchrotron Moessbauer spectroscopy. The LDA+GTB calculated phase diagram describes the experimental data. Its extension to the high temperature allows to predict metallization of the ferropericlase at the conditions of the low Earth's mantle and the metallic properties of the Earth's mantle at the depths 1400 km $< h <$ 1800 km.

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MELTING CURVES OF IONIC CRYSTALS IN QUASIHARMONIC APPROXIMATION

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Melting curves of some ionic crystals have been calculated using the density functional theory, quasiharmonic approximation and the generalized Lindemann criterion.

DIAMOND MELTING AT NEGATIVE PRESSURES

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It has been experimentally established that contact of a liquid carbon with a diamond resulted in a cracks formation in the diamond volume [1]. The graphite originate from the crack and presses on its banks with considerable force of up to 50 GPa.This treatment can lead to stretching of the diamond in the crack apex zone. Negative pressures characterizes phase transitions in this zone at ultrahigh temperatures region. Naturally, transitions has left its imprint on the structure and morphology of the final products.

Near the cavities drop-like regions were found. They contained nanographite particles. In contact with them the domains with rounded cavi-

ties were established. The carbon between the cavities had a non-graphite structure and contained of the nanodiamonds and the carbon chains. It became clear that patch in phase space under continuous tension of diamond are: the melting of the diamond at negative pressure, homogeneous nucleation of the cavities and the collapse of fluid near the boundary of it absolute stability. The analysis showed that the collapse occurred at the stage of partial coalescence of the cavities close enough to the boundary of absolute stability of the stretched liquid, as evidenced by the small crystallite size of ca. 1–2 nm was formed. Nanodiamonds and carbon chains in the products of the fracture of the fluid can be a sign of sp^3–sp structure of the liquid carbon at negative pressures.

Based on the studies performed the following tasks for molecular dynamic studies of condenced carbon at negative pressures were delivered: determination of the melting parameters of the diamond; determination of the parameters of the liquid carbon tensile rupture; comparison of the structures of liquid carbon at positive and negative pressures.

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1. The HOPG flakes were pressed to a surface of natural diamond and were melted by laser pulse with duration 0.7 ms under the pressure of 25 MPa. After that the cross sectional samples was prepared by FIB milling and was studied by the TITAN 80–300 TEM/STEM.

STUDIES OF GRAPHITE TRANSFORMATION AT COLD COMPRESSION

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The possibility of formation of new carbon phases from graphite at continuous exposure under pressures of 18 GPa to 45 GPa at room temperature was examined. Measurements were carried out in the diamond anvil cell (DAC) with electrically conductive anvils of the "rounded cone-plane" type made of synthetic polycrystalline diamonds "carbonado". The resistance measurements were carried out step by step in cycles of loading-unloading at pressure range from 18 GPa to 45 GPa. The exposure time at each fixed value of pressure was twenty four hours. The features in the pressure dependence of resistance as well as its relaxation times were found in the range 27–35 GPa. These features were referred to new phase nucle-

ation. After pressure treatment, the samples were examined by means of the workstation AURIGA CrossBeam, which is a scanning electron microscope with the possibility of X-ray microanalysis. The X-ray image of the sample subjected to the pressure of 45 GPa shows the inclusion of a new phase, which did not disappear after removal of the load. However, the new phase is poorly seen in the pressure dependence of resistivity because of shunting by a large amount of non-transformed graphite. This work was supported by the Government of the Sverdlovsk district and RFBR (grant 13-02-96039-r_ural).

CONDUCTIVITY OF DOUBLE-WALLED CARBON NANOTUBES AT PRESSURE UP TO 30 GPa

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We report the results of experimental studies DWNT bundle with the diameter of 4 nm at pressure up to 30 GPa and room temperature. Raman spectroscopy of initial sample and sample after pressure processing showed changing the ratio of the intensities of bands D/G, which characterizes the relation between the disordered and ordered structures in the sample. Disappearance of the RBM-band left peak in the Raman spectra after pressure processing took place due to destruction of the outer tube in DWNT.

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USE OF THE FEATURES IN BEHAVIOR OF A.C. ELECTRICAL PROPERTIES OF CHALCOGENIDES UNDER HIGH PRESSURE FOR ESTIMATING THE PRESSURE VALUES

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One of the features of chalcogenide materials is their ability to significantly change the electrical parameters under the applied pressure over

a wide frequency range of the electrical field [1-3]. This fact allows using these materials as working media in pressure sensors. The goal of this work is to demonstrate the possibility of using the features of the pressure dependences of the real and imaginary parts of the impedance of cells with materials based on copper and silver chalcogenides (from the systems Ag–As–S, Cu–Ge–As—Se etc.) as a physical basis for new ways of estimating the pressure value in research of condensed phases at high pressures. It has been found that if with the pressure increase at a fixed frequency of electrical field dielectric losses and the real part of the conductivity increase exponentially, then the pressure dependence of the real part of the impedance has a maximum at a certain pressure P_{max}. The appearance of this maximum was confirmed analytically [2]. The graph of the imaginary part of the impedance decreases monotonically with pressure increase and changes the direction of the concavity in the point of intersection with the graph of the real part at pressure P_{max}. The pressure P_{max} is linearly dependent on the frequency of the electrical field. Changing the frequency of the electrical field within a certain range of operating frequencies evaluated earlier for certificated materials for sensors, it is possible to provide the pressure in a certain range. The proposed method of estimating the value of pressure in the uncalibrated high-pressure chamber may be implemented by a device consisting of an *ac*-bridge and a pressure sensor which is provided with the inverter. Converter provides the ability to scan the resistance value in the neighborhood of a certain pressure and differentiation of this function to accurately determine the pressure P_{max}, when the derivative of the real part of the impedance with respect to pressure is equal to 0 and the derivative of the imaginary part of the impedance with respect to pressure is maximum.

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STUDY OF ELECTRICAL PROPERTIES OF POLYCRYSTALLINE MATERIALS ON BASED OF INDIUM AND COPPER SELENIDES UNDER HIGH PRESSURE

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Multicomponent materials from the system Cu-In-As-Se are interesting objects of investigation because under the high pressure and at the low temperature it shows the negative magnetoresistance [1].

This paper deals with the high pressure (up to 50 GPa) influence on electrical properties of polycrystalline $(InSe)_x(CuAsSe_2)_{1-x}$, $x = 0.05$, in DC and AC (1 Hz – 32 MHz) electric fields and in a transverse magnetic field $0.2 < B < 1$ T. High pressure has been achieved using the high pressure cell which detail descriptions and methods its calibration are presented in paper [2].

With increasing of pressure from 16 to 50 GPa electroresistance of the studied material decrease in DC and AC electrical fields: in DC electrical field electroresistance decrease on three orders, in AC – on one order. It was found, that studied material has a negative magnetoresistance at pressure region over 36 GPa. In pressure dependences of electroresistance measured in DC electrical field and impedance and other electrical properties measured in AC electrical field features are observed near 24 GPa and 38 GPa. The obtained results are agree with the results of paper [3] where the high pressure influence on electrical properties of materials $CuAsSe_2$ and $(GeSe)_{0.05}(CuAsSe_2)_{0.95}$ was studied.

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RESISTIVITY RELAXATION OF AMORPHOUS CHALCOGENIDES FROM THE SYSTEM Ag–Ge–As–S WITH CARBON NANOTUBES CONTENT UNDER HIGH PRESSURE UP TO 50 GPa

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Multicomponent silver chalcogenides with a silver ion conductivity are widely interesting materials because they can be applied in a huge range of devices such as memory cells, solid-state batteries, different kind of sensors etc. In order to determine how carbon nanotubes influence on physical properties of materials, glassy silver chalcogenides $AgGe_{1+x}As_{1-x}(S+CNT)_3$ with the addition of carbon nanotubes (CNT) were studied. The synthesis, atomic structure and properties of these materials having high share of ionic conductivity at ambient pressure are described in detail in [1, 2]. This study is devoted to investigation of resistivity relaxation of $AgGe_{1+x}As_{1-x}S_3$ and $AgGe_{1+x}As_{1-x}(S+CNT)_3$ ($x = 0.4$; 0.5; 0.6) at fixed pressures up to 50 GPa. Resistivity relaxation at fixed pressures above 30 GPa showed that the processes occurring in $AgGe_{1.4}As_{0.6}S_3$ and $AgGe_{1.4}As_{0.6}(S+CNT)_3$ are typical for the materials with only electron transport. The study of the electrical relaxation at fixed pressure in the range of 30 to 50 GPa showed that the resistance decreases exponentially with time for both materials. However, in the case of $AgGe_{1.4}As_{0.6}(S+CNT)_3$ the total relaxation process can be separate by both: one of them describes the relaxation processes occurring at deformation of CNTs and resulting in increasing electron conductivity, while the second may be connected with the increase in electrical conductivity during deformation and compaction of glass network with increasing static pressure. The study was supported by the Russian Foundation for Basic Research, projects 13-02-00633, 13-02-96039-r_ural_a and by the Ural Federal University development program with the financial support of young scientists.

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EFFECT OF THE EXTERNAL INFLUENCES ON ELECTRICAL PROPERTIES OF THE HIGH PRESSURE PEROVSKITE-LIKE PHASES $CaCu_3Ti_{4-x}V_xO_{12}$

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Cubic perovskite-like oxide $CaCu_3Ti_4O_{12}$ is well known as material with giant permittivity [1].The aim of this work is to investigate the effect of external influences (temperature, electric field frequency, high pressure) on the electrical properties of the high pressure perovskite-like phases $CaCu_3Ti_{4-x}V_xO_{12}$, obtained by substitution titanium for vanadium in the material $CaCu_3Ti_4O_{12}$.

The samples of compounds $CaCu_3Ti_{4-x}V_xO_{12}$, $x = 0.1$, 0.2, 0.3, 0.4, 0.5 were synthesized at high-pressure and high-temperature conditions in a toroid-type high-pressure chamber [2]. The electrical properties were studied by a method of impedance spectroscopy in the frequency range from 1 Hz to 30 MHz at the temperatures 300–600 K and at pressures 10–30 GPa (method is described in [2, 3]).

This work was supported in part by the Russian Foundation for Basic Research, projects 13-02-00633 and 15-03-00868.

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EXPERIMENTAL INVESTIGATION OF THERMOPHYSICAL PROPERTIES OF NIOBIUM AT HIGH TEMPERATURES

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Using the experimental setup for investigation of the thermophysical properties of refractory materials under high pressure and temperature a few experiments with the different metals were carried out. The experimental method is based on fast uniform heating of the small sample by current pulse. The novelty of our technique consists in the temperature

feedback heating that provides currant interruption at the desired temperature measured by pyrometer with delay less than 3 μs.

The aim of the work is to improve the accuracy of temperature measurements near the phase transition points, where the optical properties of materials change dramatically. The technique allows reaching the heating rate of 10^5 to 10^8 K s^{-1} under high static gas pressure up to several kbars.

An idea of the method consists in the rapid heating of the specimen up to the melting point in a time of 25 μs to 1 ms. Thus, through measuring the surface temperature of the sample $T(t)$, electrical current $I(t)$ and voltage drop $e(t)$ across the central part of the specimen during the experiment, one can determine temperature dependence of enthalpy $H_P(T)$, specific heat capacity $C_P(T)$ and other properties of the material.

One of advantages of our setup is a possibility of precise temperature measurement by special pyrometer [1]. It carries out the measurements in a narrow spectral band around 25 nm at the wavelengths $\lambda_1 = 0.650$ μm and $\lambda_2 = 0.900$ μm. The pyrometer has mirror field stop, which forms at the specimen surface a small area of view with the diameter of 0.3 mm. It allows using foil samples with various emitting cavities to provide thermal radiation of the sample being close to the greybody spectrum.

A high temperature investigation of such parts of the heat capacity as lattice anharmonism, electronic part and influence of equilibrium vacancies is of profound importance [2]. These factors come out mostly at the temperature region of $T_m - 100$ K in refractory metals, in particular in niobium, that is why this material has been chosen for our investigations.

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NUMERICAL SIMULATION OF THE EXPERIMENT OF ELECTRICAL EXPLOSION OF ALUMINUM FOIL

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By numerical simulation fields of pressure, density, temperature and velocity for experiment [1] were calculated. The experimental measurements have been performed on aluminum that expanded from the initial solid state by a factor of 6–9 under a supercritical pressure (> 10 kbar). Thin aluminum foil strip with thikness 10 μm sandwiched between two sapphire

plates with thikness 0.38 mm is heated by an electrical current pulse for less than 1 μs, so that the Joule heat deposited into the sample achieves 4–6 the cohesion energy. Such experimental technique ensures sufficiently homogeneous heating and practically one-dimensional expansion of the foil strip.

The results of numerical simulation and the experiment are compared. It is shown that the hydrodynamic flow in the experiment can be assumed one-dimensional. Insignificant are also elastic-plastic effects in the dynamics of aluminum foil and sapphire. The experimental and calculated pressure profiles give the same maximum pressure levels, and similar general view of the dependence of the pressure of time. It is shown that for this problem because of the small ($\sim$10 μm) of the transverse dimensions of the foil and large ($\sim$1 μs) time of measurement the thermal conductivity plays an important role. Because of the cooling of the aluminum foil surface temperature and density distributions across the aluminum sample became not homogeneous. It is important to take this fact into account for interpretation of experimental results.

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THE APPLICATION OF THE FAST PULSE HEATING METHOD FOR INVESTIGATION OF CARBON-RICH SIDE OF Zr–C PHASE DIAGRAM UNDER HIGH TEMPERATURES

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High-temperature properties of carbon and refractory carbides are of interest for the aero-space industry and nuclear technologies (a matrix of nuclear fuels). It is known that zirconium carbide is used as a protective high-temperature covering, i.e. in the form of rather thin layers.

In present work the microsecond technique of electrical pulse heating which gives uniform energy input into a film specimen is considered. ZrC+C specimens in the form of a thin layer (4.9 microns) sputtered on isolating substrates by magnetron sputtering technique were used. Specimens contained (at. %): Zr – 17.88; C – 67.69; N – 8.13; O – 5.98.

Imparted energy, resistivity (referred to the initial size of a specimen), normal spectral emissivity and specific heat were measured in the tem-

perature range of 2100 – 4500 K. The heating rate was on the order of 10^9 K/s. To obtain true temperature of the specimen the wedge-shaped blackbody design was used. The obtained results are compared with the equilibrium Zr-C phase diagram.

The solid-liquid phase transition (melting) begins at 3150 K and finishes at 3640 K. Thus the obtained temperature for the start of melting almost coincides (taking into account an uncertainty) with the temperature of the eutectic isotherm for the equilibrium phase diagram. The phase diagram shows that the composition with atomic ratio C/Zr = 3.8 (our case) corresponds to the liquidus $\sim$ 4000 K, and we obtained 3640 K. Possibly this discrepancy may be caused by large amounts of impurities.

MODELING OF NONEQULIBRIUM FIRST ORDER PHASE TRANSITION, WHICH WAS STIMULATED BY THE ACTION OF VOLUME SOURCE OF THE HEAT

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In the paper we propose a kinetic model of nonequilibrium phase transition of the first kind, stimulated by intense volume heat source on a solid surface. The results of the numerical solution of kinetic equations for nonequilibrium transition from the solid phase to the liquid phase, and the results of molecular dynamics simulations of heating and melting of the crystal are shown. When exposed to intense sources of energy to the surface of the material in the depth of the irradiated sample area is formed with an increased release of thermal energy (volume heat source). Due to the fact that in the phase transformation through each physically small volume environment takes the flow of energy from the source to the thermostat, the microvolume output from the thermal equilibrium state and acquires the ability to be bistable. Bistable kinetic model microvolume has two stable stationary state. The physical mechanism of nonequilibrium phase transition is based on the concept of the effective field ordering that occurs due to stimulated external body thermal effect and changes in the nature of the interaction energy of the atoms of the medium in the vicinity of the phase transition. To account for the propagation of heat in a medium of relaxation of the order parameter equation must be supplemented by the heat equation. Found numerical solution of kinetic

equations, theoretically found in behavior especially the order parameter and temperature versus time, of the order parameter of the temperature occurring in the vicinity of the nonequilibrium phase transition. Using the method of molecular dynamics investigated heating, melting of the crystal in a kinetic model microvolume, ie, studied the kinetics of nonequilibrium phase transition of the first kind. The simulation was performed using the program LAMMPS version 28jun14. Estimated crystals (kinetic model microvolume) was an elongated along the Z axis cuboid size $20 \times 20 \times 60$ in lattice parameters and contained ∼100,000 atoms. These studies confirmed the presence of features that occur in the vicinity of the nonequilibrium phase transition temperature, allowed to specify a quantitative estimate of the transition temperature, the temperature near the transition, time, phase transformation, so the proposed kinetic model describes nonequilibrium phase transition stimulated volume heat source.

ON DETERMINATION OF THE TRUE TEMPERATURE OF AN OPAQUE MATTER AT UNKNOWN EMISSIVITY VIA THERMAL RADIATION SPECTRUM

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Radiation thermometers are characterized by high performance and require no direct contact with the measured object. These features are of particular importance for registration of fast processes at high temperatures and for investigation of the thermophysical properties of materials. It was assumed that the spectral intensity of the free-emitted radiation and, hence, the emissivity are continuous functions of the variables wavelength and thermodynamic (true) temperature T. The object temperature is constant during the measurement process. The environment where the measured object is contained is transparent for the thermal radiation; radiation from outside is absent. The value of directional emissivity $\epsilon(\lambda, T)$ is not known. The registered radiation spectrum consisting of a intensities $I_c(\lambda_i)$ set at m wavelengths is used as an input data.

There are several approaches for determination of true temperature of opaque matters via the registered thermal radiation spectrum. Two approaches are considered.

The first approach based on relative emissivity of matter was tested and developed using the experimental data [1]. The second approach is based on temperature determination of opaque materials via the spectral

thermal radiation maximum [2]. It is shown that the area of the use of these approaches depends on the temperatures level and emissivity dependence on wavelength. It is shown that these approaches complement each other.

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CRYSTAL GROWTH MODELING USING STOCHASTIC CELLULAR AUTOMATA

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Layer-by-layer crystal growth simulation has been done in the frame of Metropolis algorithm [1]. Probability that subsequent atom will settle the empty site is defined by free area changes during surface filling which is proportional to the neighbors number. It means that the rule that governing crystal growth can be interpreted as cellular automata one [2]. During the diffusion adatom prefers to occupy nearest to step position, which determines layer-by-layer crystal growth. It has been shown that the temperature increase causes disordering of layers filling, which can be controlled by the means of mirror elastic helium atoms scattering.

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THE PROPERTIES OF THE HEXATIC PHASE IN TWO-DIMENSIONAL YUKAWA SYSTEMS (NUMERICAL SIMULATION)

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Nowadays the special focus is on the study of the thermodynamical properties of two-dimensional (2d-) systems. The analysis of the physical characteristics of these systems has not only the fundamental scientific value, but is also vital in nano- and microtechnology.

At present, there are two main approaches describing the phase transitions in these systems, based on the analysis of formation of various topological defects. The first is KTHNY (Kosterlitz-Thouless-Halperin-Nelson-Young) theory, which predicts the two-stage transition from the crystal to the liquid state of the system via the intermediate hexatic phase [1–3]. The second is GBI (Grain-Boundary-Induced melting) theory, describing the melting of a 2d-system as the first-order transition from the crystal to the liquid without the formation of the intermediate phase [4, 5].

In the present work we continue to study the phase transitions in strongly-coupled two-dimensional dissipative Yukawa systems [6]. The thermodynamic characteristics of these systems are calculated, namely the internal energy, the pressure, the specific heat and the entropy. The considered characteristics have two singular points; one of these points corresponds to the first-order phase transition from crystal to the hexatic phase, and another point corresponds to the second-order phase transition from the hexatic phase to the isotropic liquid. The dependence of the position of the melting lines and the range of existence of the hexatic phase on the concentration of the grains in the considered system is studied. The special attention is paid to the comparison of our results to the existing numerical and analytical data.

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NUMERICAL MODELING OF TORNADO-TYPE FLOWS

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There are the results of theoretical [1–3] and experimental researches [3, 4] of the destructive atmospheric vortices, such as tornadoes and tropical cyclones. There are the scheme of the emergence and sustainability of the upward vortices [1]. The theorems are proved about the existence and uniqueness of solutions for the concrete initial-boundary problems at the system equations of gas-dynamics and at the complete systems of Navier–Stokes equations. In particular, these theorems establish the conditions for the rise such flows and the direction of its rotation. There are the results of the numerical calculations the some initial-boundary problems. This results modeling the different gas flows: at the simple one-dimensional plane spiral flows to the three non-stationary flows. The times is determine from the beginning of the functioning the natural atmospheric vortices to the beginning of stationary regime. The results of the calculation agree with both the data of natural investigations of the tornado with the different parameters and the data of the laboratory experiments [3, 4]. There are the descriptions of the experimental results of group of A. Y. Varaksin (Moscow) [4] and group of S. P. Bautin (Ekaterinburg) [3]. The Varaksin's group creates and destructs the free rising swirling flows. The Bautin's group creates a bottom swirling flows, when a gas moves upwards in a vertical pipe. The experiments of both groups confirm a rise twisting and its direction when a gas moves upwards. The results of the theoretical and experimental researches verify the scheme of the emergence and sustainability of the upward vortices [1].

The study was supported by the RFBR grant 11-01-00198 and the Ministry of Education and Sciences RF project 1.8490.2013.

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NUMERICAL AND ANALYTICAL CONSTRUCTION OF APPROXIMATE SOLUTIONS OF AN INITIAL BOUNDARY VALUE PROBLEM FOR THE FULL NAVIER–STOKES EQUATIONS

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Flatsimmetric one-dimensional flow, which is the solution of the complete system of Navier–Stokes equations, constructed using infinite series of harmonics in the space variable. Used for presentation at the ends of a segment of the spatial variable slip conditions and thermal insulation. The coefficients of infinite sums have unknown functions, depending on the time. When taking into account a finite number of harmonics via parallelization calculations numerically constructed solution of the corresponding finite system of ordinary differential equations. The basic idea of parallelization is as follows: there is a control processor performing reception and transmission of data, and processors who calculates their every equation of the system of ordinary differential equations. The results of calculations.

INFLUENCE OF ARTIFICIAL VISCOSITY ON THE VORTEX CASCADE IN SHARE LAYERS

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We investigate initial stage of the onset of the turbulence in 3D free shear flow of an ideal compressible gas. In works [1,2] influence of various parameters on formation of vortex cascades is investigated. The onset and development of the vortex cascade of hydrodynamic instabilities were traced by the direct simulation of the classical laws of conservation without the influence of viscosity and walls.

The purpose of this work is to define influence of artificial viscosity on formation of vortex cascades. Viscosity was entered into system of the equations of Euler by Prandtl's approach. The results show that a small

amount of artificial viscosity of 0.001 has no effect on the rate and pattern of the vortex cascades. The increase in the value of viscosity till 0.01 slows down the formation of vortex cascades, but does not change the pattern of the flow. The value of viscosity of 0.1 has a strong stabilizing effect and the flow is not developed. Such parameters of turbulent flow as a turbulent energy spectrum, pulsations and correlations of velocity are investigated.

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SURFACE TENSION AND VISCOSITY OF NUCLEI IN LIQUID DROP MODEL

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In frame of nuclear liquid drop model an analytical solution for the frequency of capillary oscillations are obtained with taking into account the damping due to viscosity. The model has been applied for the estimation of even-even spherical nuclei surface tension σ and nuclei viscosity η. Attenuation factor γ_n to nuclear capillary oscillation frequency ω_{0n} ratio has the form:

$$\frac{\gamma_n}{\omega_{0n}} = \eta a(2n+1)\sqrt{\frac{4\pi(n-1)}{3Mn((n+2)\sigma - \frac{3Z^2e^2}{2\pi a^3(2n+1)})}}. \qquad (1)$$

where *Z, M, a and* η are the nuclear charge, mass, radius and dynamic viscosity respectively. Bethe-Weizsacker mass formula gives for σ

$$\sigma_0 = \frac{\alpha_s}{4\pi r_0^2} = 0.98\ \frac{MeV}{fm^2} \qquad (2)$$

where surface coefficient $\alpha_s = 17.8MeV$ and $r_0 = 1.2fm$.

The value of viscosity can be obtained using the quadrupole and octupole capillary frequency dependence from attenuation factors $\gamma_n \sim \eta\, n^2$, where n is multipolarity [1].

$$\eta = \frac{3}{4}\frac{M}{\pi a}\sqrt{\frac{35\omega_2^2 - 4\omega_3^2 + \frac{60E_c}{7Ma^2}}{784 - 375\beta}} \qquad (3)$$

where $\beta = \frac{\eta_2^2}{\eta_3^2}, \omega_2, \eta_2$ and ω_3, η_3 quadrupole and octupole frequencies and dynamic viscosities. For palladium nucleus Pd-106 $\omega_2 = 0.51 MeV$ ($J_P = 2^+$) and ω_3=3.9 MeV ($J^P = 3^-$), assuming that $\eta_2 \ll \eta_3$ we get $\eta = 2.82 \frac{MeV}{fm^2 c}$.

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DENSE SYSTEMS VISCOSITY

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Coefficients of diffusion and shear viscosity are calculated for the Lennard-Jones fluid and dusty plasmas. A study of the viscosity increase at the glass transition is carried out. An example of liquid aluminum is considered. Both the Einstein-Helfand and Green-Kubo relations are used. The molecular dynamics method is applied. A universal code is written, based on the analysis of particle trajectories submitted, that allows to perform calculations without a reference to the package LAMMPS.

The Lennard-Jones fluid is used to validate the code. The results for the self-diffusion and shear viscosity coefficients turn out to be similar to the other molecular dynamic simulations and to the experimental data [1].

The coefficient of shear viscosity is calculated for a model of dusty plasma. In this case, the equations of motion have a special form [2] and are not included in LAMMPS.

The embedded atom method potential is used at the simulation of the aluminum melt. The dependence of the viscosity coefficient on temperature is studied in the glass transition region. The code [3] is used, based on LAMMPS. A temperature range of the glass transition is found. The result is compared with the other glass transition criteria [3].

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RELAXATION AND TRANSPORT PROPERTIES OF LIQUID N-TRIACONTANE

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Molecular modelling is used to calculate transport properties and to study relaxation of liquid n-triacontane ($C_{30}H_{62}$). The problem is important in connection with the behavior of liquid isolators in a pre-breakdown state [1]. Two all-atom models are used: DREIDING and AA-OPLS, as well as the united-atom model TraPPE, in which three hydrogen atoms in CH_3 and two in CH_2 merge with the carbon atom; the group formed is considered as an effective point particle. Shear viscosity is calculated using the Green-Kubo formalism. In the work [2], authors use 10 quasi-independent MD runs to get statistics for the viscosity calculation. We collect statistics from a single equilibrium MD trajectory by dividing it into a number of statistically independent parts. Diffusion coefficients are calculated via the Einshtein-Smoluchowski equation. MD simulations are carried out using software package LAMMPS. The Green–Kubo method uses the stress autocorrelation function. The functions calculated appear to oscillate in the case of n-triacontane unlike for the atomic systems. Stress autocorrelation function is calculated for the liquid argon and methane (the simplest alkane) to prove this fact. Viscosity values for the both systems are obtained with a good accuracy. DREIDING potential gives correct value of the viscosity for the liquid n-triacontane, but the pressure turns out to be very high for the normal density. The value of pressure is consistent with the density in AA-OPLS model due to the Coulumb interactions and to the more complex form of the torsion interaction. The force fields are compared using the following criteria: required time for one MD step, compliance of the main physical and transport properties with experimental values. The problem of the system equilibration is considered. The TRAPPE potential is used to model the n-triacontane liquid with an initial directional orientation. The time of relaxation to the disordered system, when all the molecules orientations are randomized, are obtained. The influence of the molecules orientations on the shear viscosity value and the shear viscosity relaxation are treated.

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EXPERIMENTAL STUDIES OF BINARY MIXTURE FILTRATION IN POROUS MEDIUM

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Gas-condensate is a complex hydrocarbon mixture, which contains methane as the main component. Retrograde fluid condensation occurs in the process of gas-condensate reservoir depletion drive, i.e. liquid phase weeps during isothermal pressure decrease. A similar phenomenon prevents the further reservoir depletion, significantly reduces both the condensate recovery and the yield of gas phase, which can eventually cause a complete cessation of hydrocarbon production.

The aim of this study was investigation of hydrocarbon mixture composition influence on filtration regime of the mixture. Binary mixture "Methane + heavier componen" appeared for model mixture. The studies were conducted on the set-up "Plast" belonging to JIHT RAS, one-dimensional isothermal gas-condensate mixture flow in porous medium was simulated. Earlier on the same set-up investigation of binary mixture "methane-n-butane", acting as model of gas-condensate, had been carried out, and oscillatory flow regimes under thermobaric conditions corresponding to retrograde region at the phase diagram of the mixture had been obtained. The results of "methane-pentane" filtration investigation are represented in this paper. The second component has been chosen due to the following factors:

1. Sufficiently broad retrograde region at the phase diagram of the model mixture.
2. Set-up capability for pressure generation above critical for the model mixture.

Obtained results can find an application in new methods development of gas-condensate reservoir recovery increase.

FEATURES OF SATURATES MIXTURE FILTRATION IN POROUS MEDIUM

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Multi-phase filtration processes in porous media are naturally widespread. In this work results of methane series hydrocarbon mixture filtration research in porous media are represented. Interest of such mixtures is caused by necessary of gas-condensate extraction process increase. Gas-condensate is a valuable raw which consists of methane and its higher derivatives. Naturally oscillation flow regimes are occurred during gas-condensate recovery. The cause of these oscillations was unknown.

Our investigation has shown that filtration characteristics of such mixtures are responsible for retrograde condensation region presence at the phase diagram of the mixture. In this region liquid phase accumulation occurs under constant temperature and pressure decrease below critical. Experimental research of mixture filtration has been carried out on the set-up "Plast" disposed in JIHT RAS. Oscillation flow regime with period depending on pressure drop, mixture composition and porous medium characteristics has been discovered. Mathematical model of methane series hydrocarbon mixture filtration under constant temperature has been created. It was considered that fluid flow regime is laminar and phase pressures are equal under phase equilibrium condition (characteristic time of phase transition is far less than hydrodynamic characteristic time). The studies have shown the possibility of the self-oscillation regime existence in the process of hydrocarbon mixture filtration. Necessary condition for self-oscillations is locating the system in a retrograde region at the phase diagram. Presence of areas in which phase permeabilities are much different is the basis for implementation of the self-oscillation system feedback coupling. Self-oscillation system parameters with given porous medium properties is uniquely determined by the boundary conditions for pressure and methane mole fraction.

Consequently, some hydrocarbon mixtures (or other two-phase systems with retrograde regions) behave as a self-oscillating system in filtration process through porous medium. Account of the self-oscillation regime occurrence possibility must be taken when impact method on natural gas-condensate systems for raw yield increase is being chosen.

HYDRODYNAMICS OF HOMOGENEOUS AND MULTIPHASE FLUIDS IN A NARROW CHANNEL

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The flow peculiarities of viscous and viscoelastic homogeneous and multiphase fluids in a narrow channel are discussed by two examples. The first one is devoted to flow at the nonhomogeneous stick-slip boundary conditions initiated by the anisotropic superhydrophobic wall. This was shown to induce the helical types of flow. We found that period of the macroscopic helix of streamlines and the effective slippage length are rather sensitive to relaxation time of a fluid: the higher is the relaxation time, the larger are these flow characteristics. The dynamics of composite droplets in a narrow channel filled by a third immiscible fluid is discussed as a second example. New features of deformation behavior of such multiphase system are revealed at different ratios of core-to-shell radii, viscosities and interfacial tension.

THE FORMATION DYNAMICS OF COMPOSITE DROPLETS AND JANUS PARTICLES

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In this work, we study the interaction dynamics of two droplets of immiscible fluids suspended in the continuous liquid medium by means of numerical simulation. Two configurations of such a system are investigated: (1) the complete engulfing of one phase by another one giving a composite droplet and (2) the partial engulfing resulting in the Janus particles. The attention is focused on studying the engulfing dynamics and formation of Janus particles as functions of relative sizes, viscosities and interfacial tensions of the predator and prey droplets. The peculiarities of the engulfing dynamics at rest and shear flow are discussed.

CRITERION EVAPORATION MODELS WITH GASDYNAMICALLY PRE-FRAGMENTATION DROPS

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The basis of modern approaches designing energy plants and propulsion (EPP) for different purposes inherent mathematical modeling workflow, aimed at optimizing the parameters. One of the workflow components in the combustion chambers of the EPP is the evaporation of liquid fuel droplets. In some cases, the supply of fuel is carried out in high-enthalpy flow. In this case, the evaporation process is accompanied by a gas-dynamic acceleration and pre- fragmentation drops. Actual problem is to create a mathematical model of evaporation from the preliminary gas-dynamic pre-fragmentation fuel drops in the high-enthalpy flows. Modeling of processes heating and evaporation of the droplet is carried out by calculating the convective heat transfer. To describe the prior drop of gas-dynamic fragmentation in the used criterion equation, based on the analysis of the experimental data of other authors. Testing mathematical model in the one-dimensional formulation. The results show that with increasing gas flow rate and thus the criterion Weber We, the full time of evaporation is reduced. The path traversed by drop until complete evaporation has a maximum in the region of the gas flow velocity of 50–100 m/s. This is caused by a complex effect on the time of complete evaporation processes of fragmentation and accelerate liquid droplets, which intensified with increasing speed high-enthalpy flow. In this case, the gas flow velocity range of 50–100 m/s droplets are accelerated more rapidly than their destruction.

Calculations show that the strongest influence on the rate of gas-dynamic crushing drops has an initial value of Weber criterion. When the initial value of Weber criterion $We0 < 50$ mass loss rate drop is mainly determined by the process of evaporation, while $We0 > 50$—gas-dynamic mechanisms. At low values $We0 < 50$ a strong influence on weight loss drops have a temperature and pressure of the gas at higher We0 effect of temperature decreases and the pressure increases. To describe the processes of evaporation and pre-crushing of fuel droplets in three-dimensional unsteady gasdynamic flows a specialized module software package HyperFlow, which uses the developed mathematical model. Testing of software system and a series of calculations in relation to the challenges the organization of two-phase ignition and combustion of fuel mixtures in the

channels of variable cross-section, including the cyclical shocks. The research was supported by RFBR under grant 14-08-01118.

NEW ELECTRODE MATERIALS FOR SUPERCAPACITORS WITH AQUA AND ORGANIC ELECTROLYTES

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The study is devoted to the new carbon materials produced by thermocatalytical alkali activation of wood charcoal. Porous carbon materials play an essential role for accumulation and transfer of electrical energy. Electrochemical capacitors with double electric layer or supercapacitors (SC) belong to the most important developments in this area, and activated carbons are used as electrodes in these devices. SCs are applied in various electric power-related fields, both stationary and transportation, due to their high specific power, high charge and discharge rates and long life cycle. Carbon materials have unique features, which makes them especially lucrative as SC electrodes: high corrosion resistance, sufficient conductivity, high temperature stability, controlled specific surface and porous structure parameters. The working characteristics of carbon electrodes (specific capacity, ohmic losses) in supercapacitor are strongly influenced by the properties of porous structure. That is why investigation of the porous structure was of the great importance in this study. Limited Evaporation Technique was used to obtain desorption isotherms. Calculation of the pore size distributions from the desorption isotherms was carried out with the use of Deryagin–Broekhoff–de Boer approach and Dollimore–Heal equation within the slit-like pore model. The comparative analysis of the received pore size distributions with the electrochemical characteristics of supercapacitors allowed to determine pore ranges in which there is an effective electrical double layer formation. Electrochemical experiments were carried out to estimate the specific power and specific energy consumption for model supercapacitor cells with aqueous (4.9 M H_2SO_4) and organic (1 M TT in acetonitrile) electrolytes. Due to the opportunity to influence activated carbon structure during synthesis, rather high specific characteristics were obtained. Specific capacity around 360 F/g was obtained in supercapacitors with aqua electrolyte. Thus micropore volume of these carbons was only 0.4–0.6 cm^3/g. Supercapacitors with organic electrolyte demonstrate the capacity around 160 F/g. Micropore volume of these carbons produced special for organic electrolyte was 0.8 cm^3/g.

So it means that there is no need to create extremely high porosity to obtain high electric characteristics. The technology of thermocatalytical alkali activation of wood charcoal allows to produced activated carbons with low price and high specific electric characteristics while using them as electrode materials in supercapacitors.

EXTRAPOLATION OF IAPWS-IF97 DATA: THE SATURATION PRESSURE OF H_2O IN THE CRITICAL REGION

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Some literature sources including WEB sites are analyzed in this report. The sources contain an information about thermophysical properties of H_2O including the vapor pressure (P_s, T)-data in the form of an international standard table [1]. Our analyses shows that a traditional database [1, 2] represents these (P_s, T)-data at $t > 0.002$, here $t = (T_c - T)/T_c$ is a reduced temperature. We have considered equations $P_s(t)$ those are suggested by Wagner [1], 1973, Xiang and Tan, 1994, and Wu et al., 2005 and Abdulagatov et al., 2011. An analytical form, $F(t, D, B)$, [3] is chosen to express $\ln(P_s/P_c)$. $F(t, D, B)$ has a combined structure with scaling and regular parts: $F_{\text{scale}}(t, D, B_1)$ and $F_{\text{reg}}(t, B_2)$, here $D = (\alpha, P_c, T_c, ...)$ are critical characteristics, (B_1, B_2) are coefficients.

Adjustable coefficients $B = (B_1, B_2)$ and characteristics D are determined by fitting the combined model to input (P_s, T)-data [1] with the help of a non linear LS method [3]. Some application results are got and discussed. They include the firs and the second derivatives of $P_s(t)$ at $t = 0.00001$–0.005. We have tested some models $P_s(t)$ and compared them with $F(t, D, B)$ in the critical region. Some results mentioned are located in a WEB site http://twt.mpei.ac.ru/.

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ANGULAR DEPENDENCES OF S- AND P-POLARIZED REFLECTIVITIES OF PLASMA WITH STRONG INTERPARTICLE INTERACTION

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The investigation of properties of the electronic subsystem in a strongly correlated plasma remains an ongoing problem in the physics of high density energy. To interpret correctly the results of reflectivity measurements it is necessary to know parameters of a transitive plasma layer. Angular dependence of s- and p-polarized reflectivities at several wavelengths can be used in the integration of Maxwell equations to construct the spatial profile of the density of charge carriers.

The results of new experiments on reflectivity of polarized light on explosively driven dense xenon plasma is presented. We used a dynamic method to generate a strongly nonideal plasma, based on compression and irreversible heating of the gas in front of a high-power ionizing wave. The study of polarized reflectivity properties of strongly correlated dense plasmas have been carried out simultaneously for s- and p-polarization using laser light of frequency $\nu_{las} = 2.83{\cdot}10^{14}$ s^{-1} ($\lambda_{las} = 1064$ nm) and $\nu_{las} = 4.33{\cdot}10^{14}$ s^{-1} ($\lambda_{las} = 694$ nm) at incident angles up to $\theta = 78$ degrees and $\nu_{las} = 5.66{\cdot}10^{14}$ s^{-1} ($\lambda_{las} = 532$ nm) at incident angles up to $\theta = 65$ degrees. With density up to $\rho = 2.8$ g$\cdot$cm^{-3}, pressures up to P = 12 GPa and temperatures up to T = $3{\cdot}10^4$ K of the investigated plasma, conditions with strong Coulomb interaction (the nonideality parameter up to $\Gamma = 2.9$) were present.

The plasma composition was calculated within a chemical picture [1].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.

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PLASMA PHASE TRANSITION IN WARM DENSE HYDROGEN

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Loubeyre et al (2004) discover indications to a phase transition by optical reflectance probing at two wavelengths in a laser-driven shock wave in a hydrogen fluid sample, pre-compressed in a diamond anvil cell. Metallization of fluid molecular hydrogen is observed by Fortov et al (2007) at shock compression; resistivity decreases 4-5 orders of magnitude just in the density range where the 20 percent increase of density is demonstrated. First-order phase transition is observed in warm dense hydrogen at the pulsed-laser heating above the melting line of hydrogen at static pressures in the megabar pressure region by Silvera et al (2013).

The physical nature of the phase transition observed experimentally remains unclear. Different variants are discussed: liquid-liquid, plasma-plasma, molecular dissociation, Wigner metallization. Ab initio quantum modeling is applied in this work to elucidate the nature of the phase transition studied.

Electron density of states and the characteristic gap in it are investigated. The change of plasma frequency is suggested to be used instead of the degree of ionization to characterize the difference between two phases. Pair distribution function, and conductivity are calculated as well. Arguments are given in favor of the plasma- plasma character of the phase transition discussed. The connection is revealed with the liquid-liquid phase transition, which is observed experimentally in melts by Brazhkin et al (1989).

It is shown that Norman-Starostin (1968) ideas about (a) plasma phase transition and (b) phase diagram for fluids and liquids are not anymore hypotheses. They are confirmed by the experimental data and the new theory suggested.

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BREWSTER ANGLE OF SHOCK-COMPRESSED XENON PLASMAS

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Experimental results [1] for Brewster angle measurements are used to estimate the width of the shock front in xenon. The possible influence of the shock front width on the dense xenon reflectivity is discussed.

Dependencies of reflectivities of s- and p- polarized components (R_s and R_p) of laser radiation on the incidence angle are measured for plasma densities 2.7 and 2.8 g/cm^3 for the wavelengths $\lambda = 1064$ nm, 694 nm and 532 nm [1]. The minimum value (at the Brewster angle) of R_p is a nonzero one because the medium considered is absorptive. The ratio R_p/R_s at the Brewster angle defines the width of region of optical nonuniformity, which also can be related to the width of the wave front.

The calculated values of the Brewster angle are shifted with respect to the experimental values. It may be partially related to the nonzero width of the wave front. The estimated values of the widths are 161 nm, 154 nm, 145 nm for the wavelengths 1064 nm, 694 nm and 532 nm respectively. These values are obtained in the framework of the Drude theory of reflection in optically nonuniform media. The density functional theory is applied to calculate values of the dielectric function and refraction. The satisfactory agreement of theoretical results with the experiment is obtained for the wave front width 200 nm in the framework of Drude model [2].

The assumption that the width of the shock front could improve the agreement of the Drude formula with static collisional frequency with the experimental data is introduced in [3] for the normal incidence of laser radiation. However the suggested width of the wave front is approximately 800 nm, which considerably exceeds both theoretical estimations 100 nm and the results obtained in this work. The effect is discussed if the widths found could influence the normal reflectivity obtained in the framework of the density functional theory [4].

The work is partially supported by the RAS Presidium program of the fundamental investigations No 2 Matter at High Energy Densities.

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ONE-ELECTRON MODEL OF THE HIGH-FREQUENCY DIELECTRIC PERMEABILITY OF DENSE PLASMAS

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The approach is developed to calculate reflectivity and high-frequency dielectric permeability of dense plasmas. The Kubo-Greenwood formula is applied. One-electron wave functions are used.

Plane waves are substituted for the wave functions of the free states. Hydrogen-like wave functions are substituted for the wave functions of the bound states. Effective principle quantum numbers are used to take into account the difference of the atom from the hydrogen atom. The restriction of the excited pair bound states is included in the calculations. The boundary energy is found from the molecular dynamics simulations earlier as $E < -2(4\pi/3)^{1/3}e^2 n_e^{1/3}[Z/Z_{av}^{1/3}]$.

Calculations are performed for the shock-compressed xenon. The results are in the fair agreement with the experimental data [1] for densities $\rho > 2g/sm^3$ whereas the remarkable discrepancy appears at low densities.

On the one hand, the discrepancy can be attributed to a finite width of the shock front. The width increases with the decrease of density and can contribute to the reflectivity at low densities.

On the other hand, the approximations used for the wave functions are rather rough. The number of excited states, which are necessary to include into calculations, increases with the decrease of the density. It is another source of the error to be removed at low densities.

The work is partially supported by the RAS Presidium program of the fundamental investigations No 2 Matter at High Energy Densities.

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THERMODYNAMICS OF NEWTON–WIGNER RELATIVISTIC PARTICLE IN EXTERNAL POTENTIAL FIELD

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The work covers simulation of thermodynamical properties, such average energy and heat capacity, of relativistic Newton-Wigner pseudoparticle [1], which is placed in external potential feld. Spinless Newton-Wigner pseudoparticle corresponds to solutions of relativistic wave equation (Klein-Gordon equation) with positive energies [2]:

$$\left[\left(i\hbar\frac{\partial}{\partial t} - eA^0(\mathbf{x})\right)^2 - c^2\left(-i\hbar\nabla - \frac{e}{c}\mathbf{A}(\mathbf{x})\right)^2 - m^2c^4\right]\phi(\mathbf{x},t) = 0.$$

where A_0 is scalar, and (A_x, A_y, A_z) - vector potential of external feld. In this work we have made generalization of Wiener path integrals for thermodynamics [3] on relativistic Newton-Wigner pseudoparticles. Also, we have developed quantum Monte-Carlo procedure for calculations of thermodynamical averages. For demonstration of the procedure, we have calculated average energy and heat capacity of spinless Newton-Wigner pseudoparticle in $1D$ - harmonic potential. Such system, which can be named as relativistic harmonic oscillator, is defned by Hamiltonian:

$$\hat{H} = \omega(\hat{p}) + \frac{m\omega^2}{2}\hat{x}^2$$

where m is mass of particle, ω is oscillator parameter.

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THE ELECTRONIC TRANSPORT COEFFICIENTS AND PRESSURE OF Ni PLASMA

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The thermophysical properties of various substances have been studied for more than a century because of their importance in fundamental tasks and applications. Among these properties there are the pressure, the electrical and thermal conductivities etc. However at high temperatures ($T > 5$ kK) there is the deficiency of corresponding information as far as it is difficult to carry out the measurements in these region. Nevertheless, recently the new experiments for these properties have appeared in the plasma region [1-4]. So the existing theoretical models can be checked.

In our previous works [5-7], we have developed the model to calculate the chemical composition, electronic transport coefficient, pressure, internal energy for the plasma under study. Here we have applied the chemical model, developed earlier for various substances, to obtain the plasma composition of Nickel. So we modified it correspondingly. The pressure and internal energy can also be obtained by means of this technique. The coefficients were calculated within the relaxation time approach (also the BGK approximation [8]). The range of applicability of both approaches is limited when the density increases (see corresponding estimates in [6, 7]). But the measurement data [1-4] are located in the area where the application of our approach is still correct. Previously our model has been successfully applied for plasmas of noble gases, noble metals, silicon and boron [5-7]. Here we use it to study Nickel. The measurements of the properties under study are presented in [1, 2] at $T \geq 10$ kK and densities less than normal one. Our calculations have also been carried out under these conditions. The obtained results are in good agreement with the results of measurements and calculations of other authors.

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MODEL FOR DESCRIBING NON-EQUILIBRIUM HELIUM PLASMA ENERGY LEVEL POPULATION

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The fact that helium plasma at atmospheric pressure at temperatures from 1 to 5 eV is in non-equilibrium state has been noted by various authors. The necessity to use special methods is noted in [2] where an elaborate collisional-ionizational model is described allowing to make a more detailed description of excited level structure and of transitions between them. Such approaches had been suggested in earlier works as well [3], but on a lower qualitative level because complex calculations of speeds of a multitude of processes were an impossible task for computers at that time. However, now this approach appears to be rather feasible. In order to analyse the structure of helium plasma excited level population, a system of equations derived from non-stationary model will be solved without using approximate solutions [1, 3], using a possible minimum of approximations found in [2] and using experimental data on cross-sections and process speeds where possible. Our system of equations includes all energy levels found in [4] for atoms and ions. The concentrations of charged particles are be found through the solution of equations of process kinetics in which they are used as unknown variables instead of using Saha equations. The challenge is to find roots of the system of 113 non-linear equations (the number of excited states and auxiliary equations). The tests run on a system of 17 equations including a part of excited levels have shown that is impossible to obtain a correct solution using double precision (64-bit) arithmetics due to its extreme stiffness. The values on which iterative procedures converges are affected by representation and round-off errors to such extent that substituting them back into the equations yields inagreement of a magnitude comparable to that of the found values themselves. To solve the systems with better precision, Maple software was used.

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RADIOPHYSICAL METHODS OF MODELING THE ELECTROMAGNETIC WAVES PROPAGATION THROUGH A FLAT PLASMA LAYER

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This paper presents the model variants of plasma layer creating by microwave discharges and plasma jet sources. Methods of creation a model quasi-dynamic plasma antenna on the basis of plasma jet and antenna type plasma structures of microwave range are also considered.

Pulsed discharge in a capillary with ablative wall can be used as a method of creating plasma antenna. A microwave discharge is another perspective method for plasma antennas creation in centimeter-decimeter wavelengths range that allows us to apply this approach for modeling different types of plasma antennas (dipole, traveling wave antenna, spiral antenna, and others).

Numerical modeling was initiated to analyze the interaction of microwave radiation with plasma layer. It is assumed that 2D consideration will allow investigating the influence of various types of regular spatial plasma structures on the characteristics of the transmission and scattering of EM waves beams. The model allows to investigate also the development of MW plasma structures (it is virtually impossible to implement in the framework of 3D modeling).

A TECHNIQUE FOR THE RADAR CROSS-SECTION ESTIMATION OF AXISYMMETRIC PLASMOID

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The existing simulation codes of the radar cross-section estimation are developed for fixed shape objects therefore these codes cannot be used for inhomogeneous plasmoid because the shape of the wave reflection surface depends on the angle between the plasmoid axis and the wave vector. This paper presents simplified model for the radio waves backscattering

from axisymmetric plasmoid. The model developed is based on Huygens's principle. According to physical optics method, the electrical current on the reflection surface is a source of waves scattered from reflecting plasma. This surface is approximated by a set of simple surfaces – a sphere, a cylinder and a cone. This assumption facilitates the summation of elementary scattered waves and the angular coordinate integration can be made analytically in closed form. As the result the field of scattered wave is given by the sum of longitudinal integrations. The radio waves scattering from penetrable plasma is caused by the electron oscillations in the electromagnetic wave field. For axisymmetric penetrable plasma the angular coordinate integration can be made analytically therefore the field of scattered wave is given by double integral. The approach developed takes into account the radio waves backscattering from both penetrable plasma and reflecting plasma and reduces the radar cross-section estimation to numerical integrations. The computer program on the basis of MATLAB is developed for the radar cross-section estimation. In this way it is easy to use tabulated data for the electron concentration and the collision frequency.

NUMERICAL SIMULATIONS OF HEAT AND MASS TRANSFER AT ABLATING SURFACE IN HYPERSONIC FLOW

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In this paper numerical modeling of heat and mass transfer in 3D hypersonic flow is presented taking into account Thermal Protection System destruction.

The simulation method is based on numerical solution of three-dimensional heat equation within TPS, calculation of heat- and mass flux on the flow-wall interface, estimation of the surface recession rate, and re-shaping of both surface and interior. Ansys Fluent is used for solving the heat problem, which is capable of working on unstructured grids.

For validation of the developed method 3D unsteady numerical simulation of thermal state within a sphere-cone shaped hypersonic vehicle was carried out. Data on hypersonic flow necessary for the surface model were taken from the calculations done with JIHT RAN PlasmAero code. Unstructured tetrahedral mesh with about of 100,000 grid cells was used for this test. Time-dependent temperature and heat flux fields were cal-

culated. As well, surface recession rate and body re-shaping was assessed in calculations.

COMPUTATIONAL GAS DYNAMICS IN A WIDE RANGE OF MACH NUMBER ON HETEROGENEOUS CLUSTER ARCHITECTURE

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The specific features of numerical method for gas dynamics problems are considered in this paper. The viscous flows are considered in a wide range of Mach number. The numerical method is based on conservation laws applied on unstructured heterogeneous mesh with further integration on complex cluster architectures. Mesh generating software is non-commercial GPL-licensed, namely GMSH and Salome. Boundary layers are meshed by prisms or with hexahedra with further adaptation to tetrahedral using prisms. Application of unstructured mesh allows one to perform calculation of geometrically complex 3D objects with strict conservation properties, unlike immersed boundary methods. The developed numerical method includes multiple flux solvers (Godunov's, HLLC, Roe-Fix, AUSM, etc.), first and second order spatial approximation, explicit, semi-implicit or implicit first order time schemes. The heterogeneous computational environment developed by the authors is used in order to perform computations. The program is written for heterogeneous cluster architecture under UNIX OS using OOP C++ with CUDA extension. The main computational module is an NVIDIA GPU. Main advantage of the GPU utilization is the increase of the efficiency of a single computational module, thus greatly decreasing load on the cluster's interconnect. A wide range of problems is used for verification of the developed computational complex. Subsonic internal swirling flow in a pipe and hypersonic flow problems with different body shapes are considered. All results on these problems had a good agreement with reference data. Benchmarking performance was conducted on subsonic and hypersonic problems, the lesser result was chosen. Explicit method has almost linear acceleration on 5 GPUs. Fully implicit method has 76% of linear acceleration on the same 5 GPUs cluster. The performance of implicit method on five GPUs is about 3.4 TFLOPS, estimated by the nvprof program.

INVESTIGATION OF TORCH FROM ARGON AND NITROGEN PLASMA GENERATOR WITH ELECTRICAL PROBE

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Relative simplicity and compactness of probe measurement allow using it under onboard conditions, for example, on descent spacecraft. In this case the probe technique can be useful for measurement of plasma frequency that occurs behind the bow shock at the altitude from 100 km and above. The plasma formation near the surface results in several negative consequences such as heat shielding destruction, partially absorption or full screening of telemetric, video, voice MW-signals [1]. For example, last of mentioned phenomena is concerned with such plasma parameter as plasma frequency and its value depends on electron concentration directly.

This work is devoted to investigations of plasma of plasmatron (plasma generator) torch by mean of probe technique, the parameters of that are close to plasma parameters that occurs near the surface of descent spacecraft under the movement at the Earth atmosphere. The probe measurements of electro-conductivity have been performed by means of volt-ampere characteristics for nitrogen and argon plasmas, with their temperatures and electron concentration being similar to those of the plasma behind a bow shock wave of a descent spacecraft [1]. The numerical calculations of plasma parameters (electro-conductivity, electron concentration) are carried out for nitrogen and argon in dependence on temperature. Using the torch plasmatron with argon and nitrogen as an example, approbation of the proposed technique is performed with local plasma parameters properly obtained.

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COLD DARK MATTER AND DARK ENERGY IN UNIVERSE: POSSIBLE ANISOTROPY OF THE EARTH OBSERVATIONS

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The $\Lambda - CDM$ standard model of Big Bang cosmology looks formally very successful, but it includes two vastly dominating and unknown - directly unobserved - components, Cold Dark Matter (CDM) and Dark Energy (DE), filling more than 95 percent of the Universe. The hypothesis of antigravitational interaction of elementary particles and antiparticles has been developed in [1] for the simple two-component hydrodynamic model with gravitational repulsion and attraction. An increase in the Jeans instability rate, the presence of antiscreening, and the dominant role of the gravitational repulsion as a possible mechanism of spatial separation of matter and antimatter in the Universe are shown, as well as the observable acceleration of far galaxies. The suggested approach permits to reestablish the idea about baryon symmetry of the Universe, causing its steady large-scale flatness and accelerated Universe expansion. On the basis of the above hypothesis and results in this presentation one can assert that the Euclidian geometry can be used for the Universe large-scale evolution description after the Big-Bang. This statement leads to the conclusion about existence of the anisotropic observable effects (as the red shifts and some other) in astronomical observations.

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ON THE AXIAL AND TRANSVERSE COOLING RATES OF AN ANTIPROTON IN POSITRON GAS IN STRONG MAGNETIC FIELD

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In the experiments in CERN antihydrogen is formed during mixing of antiprotons and positrons. One of the main goals of these experiments is obtaining sufficient quantity of anitH atoms to find possible differencies in antiH and H spectra. To trap antiH atoms a magnetic trap with depth of about 1K is used. But initial kinetic energies of antiprotons are much higher - from 100K to tens of eV. This represents a problem because formed atoms have kinetic energy of antiprotons since high mass ratio of antiproton and positron. Antiprotons can be cooled during collisions with positrons since positron energy is about 10K and number of positrons is 50 times greater than number of antiprotons. But the question here is what process is faster - atoms formation during threebody recombination or antiproton energy relaxation. Theoretical investigation of the processes is complicated by the presense of strong magnetic field of magnitude of 1-3 Tesla. Because of that numerical study of relaxation of the antiproton energy in positron gas was performed using molecular dynamics method. Calculations were made for different values of particles density and energy and magnetic field magnitude. It is shown that the relaxation rates of parallel and perpendicular to the direction of magnetic field antiproton velocity components are different. Parallel relaxation rate is much less than perpendicular. The difference increases with the increase of the magnetic field magnitude and may be up to 10 times for the experimental conditions. Due to the slow relaxation of the parallel velocity the recombination may occur when parallel velocity is still high. This may result in high antiatom axial velocity and made it impossible to trap antiatoms in the existing experimental conditions. Some experiment results have implications that axial velocity components of antiatoms are indeed much higher than transverse components.

Calculations were performed on MVS-100K supercomputer of Joint Supercomputer Center of RAS (mvs100k.jscc.ru)

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EXPERIMENTAL TECHNIQUES AND NUMERICAL SIMULATIONS FOR STUDY OF RYDBERG MATTER AND ULTRACOLD PLASMA

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We will present a short review of our recent experimental and theoretical results. A new experimental technique for precise measurements of Rydberg state's energies of Li7 has been developed [1]. The experimental setup includes magneto-optical trap and powerful continuous wave UV laser system. The diagnostic of Rydberg states has been performed by direct observation of resonance fluorescence of ultracold lithium atoms in magneto optical trap.

The boundary of phase equilibrium in the frame of pseudo potential model of ultracold plasma was investigated [2]. By using Monte-Carlo method a curve of phase equilibrium is calculated for basic pseudo potential model of ultracold plasma. A value of critical point was defined. Correlations functions around the curve of phase equilibrium is calculated as for a gas part as for a liquid part of binodal. The correlators for heavy charged particles in magnetic field are calculated by using molecular dynamic method. The thermalization times are defined. For antiprotons and positrons the energy correlators and decay constants for the field B = 1.5 Tesla are obtained when magnetic field is parallel and orthogonal to the particle velocity. The energy losses in the direction of the magnetic field are remarkably less than in the perpendicular direction.

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TWO-PHOTON EXCITATION OF ULTRACOLD ATOMS TO RYDBERG STATES

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In this work we discuss two-photon excitation and diagnostic of ultracold Rydberg atoms in a magneto-optical trap [1]. Lithium atoms were excited by using ultraviolet CW laser. For identification of Rydberg transitions we recorded resonance fluorescence of ultracold atoms. Spectra of transitions 2P — nS, 2p — nD were measured. Our results are in good agreement with theoretical simulations and experimental data available in literature. Presented work is a part of our project focused on preparation and study of ultracold plasma and Rydberg matter [2, 3].

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IDENTIFICATIONS OF RYDBERG TRANSITIONS IN ULTRACOLD LITHIUM ATOMS USING PRECISE WAVEMETER

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In our laboratory is developed a simple technique for identification and measurements of Rydberg transitions. In our experiment the frequency of the ultraviolet tunable laser was controlled with precise wavemeter Angstrom WS-U. The wavemeter was calibrated by using laser locked to Doppler-free absorption resonance in rubidium 85 vapor cell. Ultracold lithium atoms were trapped in magneto-optical trap by cooling lasers

tuned to resonance transitions 671 nm [1]. The atoms were excited to Rydberg states by using CW ultraviolet laser (wavelength near 350 nm) [2]. When the frequency of UV tunable laser coincided with frequency of Rydberg transition, the resonance fluorescence of ultracold atoms decreased. This work was supported by the MK-4092.2014.2, NSh-6614.2014.2, the RFBR 14-02-00828, the Presidium of the RAS (Basic Research Program "Investigation of Matter in Extreme States" headed by V.E. Fortov).

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CALCULATING THERMODYNAMICAL PROPERTIES OF TWO COMPONENT "SHELF COULOMB" PLASMA MODEL USING GIBBS STATISTICAL ENSEMBLE MONTE CARLO TECHNIQUE

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Earlier [1] a two-component plasma model, which we called a "shelf Coulomb" model has been developed. A Monte Carlo study for canonical NVT ensemble with periodic boundary conditions has been undertaken to calculate equations of state, pair distribution functions, internal energies, and other thermodynamical properties of the model. Now for the first time the attempt is made to utilize so called statistical Gibbs ensemble Monte-Carlo technique for this model. The Gibbs enseble technique was proposed by Athanassios Z. Panagiotopoulos back in 1980-s [2] and is now commonly used for obtaining the phase behavior of one and many components fluids and mixtures. The goals of this work is to investigate the applicability of Gibbs ensemble method to plasma "shelf Coulomb" model and to verify results for equilibrium and phase properties obtained using NVT canonical ensemble technique. First simulations show qualitatively similar results for critical point region for both methods. And yet much remains to be calculated and discussed. This work is supported by Russian Science Fund grant (RNF 14-19-01492).

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KINETIC CHARACTERISTICS OF THE MAGNETO-OPTICAL TRAP

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For investigation of ultracold plasma recombination in strong magnetic field it is necessarily to load the ground-state atoms in a dipole trap. In order to increase a number of trapped atoms, the temperature of the loaded atoms have to be less than the Doppler-limit. In our presentation we will discuss possible techniques of sub-Doppler cooling of lithium atoms and accurate temperature measurements [1]. Also we will discuss different methods of loading atoms in dipole trap. In order to study the recombination of ultracold plasma a special water cooled magnet system (0.1 Tesla) is developed.

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KINETICS OF EXCITED INERT GAS ATOMS IN A GAS DISCHARGE PLASMA

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A gas discharge plasma is a nonequilibrium system in principle [1–3] because first an electric field energy is injected in a gas through plasma electrons and then electrons transfer this energy to atoms. Hence, this system requires the kinetic description [4] which is based on the cross sections and rate constants of elementary processes. A general approach to this problem [5, 6] is based on the simultaneous analysis of the kinetic equation for the energy distribution function of electrons and the balance equations for excited atoms based on parameters of elementary processes in a gas discharge plasma. Usually, elastic and inelastic collisions are of importance for kinetics of a gas discharge plasma, and the peculiarity of this description is such that the theory does not allow to evaluate the cross

sections of electron-atom processes reliably, so that experimental data are required for this goal or certain scaling models based on experimental results.

Now there are a lot of computer simulations based on this approach but all those are not reliable for two reasons. First, processes of formation of fast electrons and excited atoms have the self-consistent character, that is the process of atom excitation leads to a sharply drop of the electron distribution function with an increasing electron energy, and this in turn causes a decrease of the excitation rate. In this paper the coupling of these processes is taken into account for an inert gas discharge plasma with a not large electron number density ($N_e < 10^{13} cm^{-3}$). Second, the fact of the dependence of the atom excitation cross section on the electron energy accounts for in this paper by based on the quenching rate constants which are independent of the electron energy at low energies.

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MEASUREMENT OF ION ENERGY LOSSES IN GAS-DISCHARGE PLASMA

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The studying of stopping processes of heavy charged particles in the plasma relates to the fundamental problems of plasma physics and the physics of high energy density in matter. In recent years, researches on the interaction of ion beams with plasma actively was carried out in many scientific centers of the world: Germany, France, USA, Japan and China. However, the experimental data on the interaction of ions with the plasma at energies of particles in the range of 40 - 500 keV / amu are almost absent. Thus, the study of the processes that determine the energy loss of ions in the plasma, have acquired great importance. Within the solving

the fundamental problem and developing of methods, a series of stopping experiments on the accelerator based in IMP (Lanchou, China) was provided. Also the discharge of plasma target device was diagnosed in ITEP in cooperation with specialists from MEPhI. High-current discharge target device [1], created in ITEP was installed and started on the test stand in IMP CAS, Lanzhou. Current discharge parameters in the target was measured. High current pulse generator produce potential difference of 2 to 5 kV, and initiates a gas discharge in a hydrogen gas at a pressure of from 1 to 10 mbar. The characteristic value of the discharge current is 1.5 kA at full pulse duration 10 ms. Parameters of the plasma generated in the target have been measured [2]. The linear density of the plasma electrons is in the range of 4*10$\hat{}$17 cm$\hat{}$-2 to 1.31*10$\hat{}$18 cm$\hat{}$-2, depending on the initial values of the discharge voltage and the gas pressure in a cold target. The maximum degree of ionization of the plasma in the target was obtained as 0,62 +/- 0,05 at the value of the initial gas pressure of 1.5 mbar. Stopping experiments of protons and helium ions (He + 1 + No 2) with an energy of 100 to 200 keV in plasma targets device at different discharge parameters was produced. [3] Works are performed with assistance of the Russian Foundation of Basic Research (grant No. 12-02-91186-GFEN A)

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RADIATIVE SPECTRA OF DENSE HYDROGENIC PLASMA: LINE-TO-CONTINUUM TRANSITION PROBLEM

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The problem of reasonable description of the line-to-continuum transition in radiative spectra has been discussed during many decades. While the isolated atom theory shows a smooth transition, a number of computation problems appear in practical calculations (for example, the line wing extension over the continuum threshold) because of the lines and continuum are considered in different ways. The line broadening theory takes into account the density (non-ideality) effects, while the continuum is usu-

ally calculated in the ideal plasma approximation. Therefore, the problem of the matching of discrete and continuum spectra arises. At the present, the method of effective populations (or occupation probability method) is normally applied for the matching. It assumes that the intensity of the high members of spectral line series decreases in proportional to the occupation probability factor W due to the destruction of the higher excited levels in plasma microfields. Then the lost of the line oscillator strength is compensated by the continuum expansion to the near-threshold region with a factor $1-W$. We have presented more natural alternative approach in the framework of which the line and continuous spectra are calculated using the same model. We consider a hydrogen atom (hydrogen-like ion) immersed in quasistatic ion microfield approximated by a homogeneous (in atomic scale) electric field, and make the calculation in parabolic coordinates. Then the radiative spectrum is a continuum with Stark resonances corresponding to the region below the potential barrier top. After averaging over quasistatic microfields with corresponding distribution function and inclusion of the electron broadening of the Stark resonances we obtain the radiative spectrum of hydrogen plasma containing the lines and continuum. Calculations for conditions corresponding to recent experiments on dense hydrogenic plasma radiation show a good agreement with experimental data. Moreover, in a sense our method can be considered as a justification of the occupation probability method.

THE ELECTROSTATIC INTERACTION OF TWO CHARGES IN EQUILIBRIUM PLASMAS WITHIN THE DEBYE APPROXIMATION

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In paper [1], on the basis of the analysis of the force between two macroparticles in a plasma by using the Maxwell stress tensor it was shown that within the Poisson – Boltzmann model two macroparticles with the same charge always repulsed each other in both isothermal and nonisothermal plasmas. Ignatov in [2] deduced the same result. In spite of this clear conclusion new papers are regularly published with the statement of the same charged particle attraction in the equilibrium plasma (see, for example, papers [3–5]). This paper is devoted to a careful study of two charge interaction in the equilibrium plasma within the Debye approximation. The interaction potential is obtained in both the grand canonical

and canonical ensembles. The effect of outer boundary conditions for the electric field strength and potential on the electrostatic force is studied.

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CHARACTERISTICS OF THE DISCHARGE FOR HIGH RATE DC MAGNETRON SPUTTERING

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The work aims to study the features of gas discharge plasma used for high-rate sputtering processes for structural and functional coating production. A DC magnetron sputtering of copper target was carried out in argon plasma at an average power density from 10^1 to 10^2 W/cm^2. Current-voltage and current-pressure characteristics of the magnetron discharge in the buffer gas pressure range from 1 to 30 mTorr were measured. The intensity profiles of integral glow discharge and the optical emission spectra were obtained. A Monte Carlo model was developed for calculating the trajectories of electrons in crossed electric and magnetic fields (ExB), taking into account elastic and inelastic collisions of electrons with atoms of the buffer gas. For a number of typical values of the magnetic induction and electric potential the spatial distribution of ionization coefficients and excited electronic states of argon were calculated. The calculation results are consistent with the optical emission data.

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MICROPARTICLE CHARGING IN A DRY AIR PLASMA CREATED BY AN EXTERNAL IONIZATION SOURCE

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In the present work the dust particle charging is studied in a dry air plasma created by an external ionization source. The ionization rate is changed in the range 10^1–10^{20} $\mathrm{cm}^{-3}\mathrm{s}^{-1}$. The main ion components of the plasma are obtained by the analysis of ion-molecular reactions from [1]. It is found that the main positive ion is O_4^+ and the main negative ions are O_2^- and O_4^-. The point sink model based on the diffusion-drift approach [2] shows that the screening potential distribution around a dust particle is a superposition of four exponentials with four different spatial scales. The first scale almost coincides with the Debye radius. The second one is the distance, passed by positive and negative plasma components due to ambipolar diffusion over their characteristic recombination time. The third one is defined by the negative ion conversion and diffusion. The fourth scale is described by the electron attachment, recombination and diffusion at low gas ionization rates and by the recombination and diffusion of negative diatomic ions at high ionization rates. It is also shown that the electron flux controls the microparticle charge at high ionization rates despite the electron density is much less than the ion one.

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STRUCTURE AND PROPERTIES OF THE CERAMICS BASED ON THE COMPOSITION POWDERS FROM DUSTY PLASMA

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Using the plasma methods of particle surface processing we obtain the composite ceramics with improved performance data. The composite ceramics may be required in the production of functional materials for chemical and radiation-aggressive environments, structural elements for high pressures and temperatures in neutron diffraction studies of materials under these conditions, tool products. To incorporate homogeneously a small amount of binding material or modifying agent in the batch consisting of micron size particles is a problem of composite material production process. In this work the problem is solved by deposition of a thin coating on the initial powder particles by means of high-rate magnetron sputtering. The confinement of dusty particles in plasma was used in fine powder processing procedure.

Composite powders based on some materials were obtained: consisting of diamond particles with cobalt coating and of the Al-Cu-Fe quasicrystalline particles with nickel one. The composition of the obtained composite powder, structure and mechanical properties of compacts obtained by sintering at high pressure and temperature were studied. The results showed that the method provides sufficiently high uniformity incorporation of small quantities of additives (at concentration of about 3 wt. %) to fine powders. The conditions of sintering which provide producing compacts with improved performance data from the composition powders were established. The diamond compacts showed high densities and high elastic moduli. The quasicrystall based ceramics showed low friction coefficient and low wear. The noted material properties were provided by the complex of the methods used.

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DETERMINATION OF THE CHARGE AND THE MASS OF A SINGLE MICROPARTICLE IN THE ELECTRODYNAMIC TRAP

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The electric charge of the microparticles is a fundamental characteristic that determines the particles behavior in various processes. The known experimental methods of the charge determination require a selection of the particles from the flow and complex electrical measurements [1].

The using of the electrodynamic quadrupole trap allows to performing the charge measurement without selection of microparticles from the flow. In this work, we measured the charge and the mass of the individual Al_2O_3 particle, confined in the electrodynamic trap.

The electrodynamic trap was formed by four steel, vertically oriented electrodes with diameter d = 4 mm, set in the corners of a square with sides of 3 cm. The length of the electrodes was equal to 31 cm. To the electrodes the AC 50 Hz voltage with amplitude of 4kV was applied. On the axis of symmetry of the trap the steel ball with a diameter D = 8 mm was installed. The ball was placed on a 12 cm length metal rod. To the ball the constant electric potential was applied.

The mass of the particle was determined by its free-fall velocity. From the structure of particles confined by the electrodynamic trap all particles except one were removed. The potential U = 4 kV to the ball was applied. Thereafter, the ball was grounded, and the particle begins to fall under gravity. The trajectory was recorded with a video camera.

To determine the particle charge, the distance between the particle and the ball was measured. The weight of the particle was counterbalanced by the force acting on the particle by the electric field.

The measured values of the particle charge were in the range of $3 \cdot 10^5$ – $3 \cdot 10^6$ e. The measured values of the particle mass were in the range of $2 \cdot 10^{-11}$ – $5 \cdot 10^{-10}$ kg.

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EFFECTIVE FORCES AND PSEUDOPOTENTIAL WELLS AND BARRIERS IN THE LINEAR PAUL TRAP

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The effect of charged microparticles trapping in an alternating electric field is used in Paul trap devices. The alternating electric field in the trap is generated by alternating voltage of specific frequency that is applied to the trap electrodes. Such alternating electric field may result in arising of a pseudopotential well or barrier in various areas of the trap.

The theory of motion of nonrelativistic charged particle in an alternating electric field was developed in [1]. An effective force acting a charged particle is called Gaponov-Miller force [2]. The generalizations of the theory of charged particle motion in an alternating electric field in gaseous medium with the friction force proportional to the particle velocity was derived in [3].

The purpose of this work is to study effective forces acting on a charged micropaticle and identification of areas of pseudopotential well or hill. The equation of microparticle motion is solved for this purpose: $m_p\ddot{\vec{r}} = m_p\vec{g} + \sum_i(\vec{E_i}(r)q_p sin(\omega t+\phi))+6\pi\eta r_p(\vec{v_f}-\dot{\vec{r}})$ where m_p is microparticle mass, $\ddot{\vec{r}}$, $\dot{\vec{r}}$ and $\vec{r}$ are microparticle acceleration, speed and radius vector respectively, $\vec{g}$ is free fall acceleration, $E_i(r)$ is electric field intensity for electrode i, q_p is microparticle charge, ω is alternating field frequency, ϕ is phase shift, η is dynamic viscosity of gas medium, r_p is microparticle radius, v_f is speed of gas.

The effective force acting the charged microparticle is calculated by equation $F_{eff} = -\bigtriangledown\overline{W}$ where $\overline{W} = \frac{1}{2}m_p\overline{\dot{r}^2}$ is averaged over the period of oscillation kinetic energy.

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CONFINEMENT OF CHARGED MICROPARTICLES IN A GAS FLOW BY THE LINEAR PAUL TRAP

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Charged dust particles (microparticles) are often present in many power installations where they can play a positive or negative role. As an example let us mention installations of plasma etching in which the formed particles are to be removed as well as in the fusion devices. But there are problems when it is necessary to remove particles of definite sizes that is not possible to achieve with the help of electrostatic precipitators using the direct current corona discharge. In the previous works [1, 2] we demonstrated a possibility to confine the Coulomb systems of charged microparticles in the atmospheric pressure air with the help of the electrodynamical traps. We have determined the regions of a confinement of charged microparticles in a wide range of parameters (charge, mass, radius of microparticles, electric field strength and its frequency). To capture and confine charged microparticles in a gas flow the updated electrodynamical trap has been suggested [3]. The aim of the present work was the experimental study of a possibility to confine charged microparticles in the linear Paul trap in a gas flow. The possibility to confine charged microparticles in a gas flow using the linear Paul trap was confirmed experimentally.

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THE LOW FREQUENCY OSCILLATIONS OF DC DISCHARGES WITH DUST PARTICLES

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Collective processes in dusty plasmas can lead to the development of instability associated with loss of plasma energy on dust particles. The intermittent mode with the development of self-oscillations of the discharge was previously observed in the dc glow discharge in air with dust particles [1]. In this study is discussed the unstable mode of dc glow discharge characterized by low-frequency glow pulsations observed in neon dusty plasma. The pulsing mode of discharge is associated with a change in the current-voltage characteristics (CVC) of the discharge. The discharge oscillations are determined by transitions between the normal and subnormal discharge regimes and correspond to the different dynamics of dust particles. This type of instability is characterized by a negative differential resistance. Such a shift to position along CVC with less value of discharge current, can be accompanied by the transition from the stationary state of striations to the state with moving striations. The mode with moving striations is known to be accompanied by oscillations and waves in dusty plasma, which reduce the plasma losses and may contribute to a return to the initial mode of discharge. Such instability is the result of uniform energy dissipation in a plasma bulk. It is determined by the particles dynamics and depends of the number density (or the number) of dust particles [2]. In the initial state, the dust particles are positioned in the center of the discharge tube with a maximum number density. The moment of transition between modes of discharge is accompanied by radial expansion of the dust cloud. The dispersion of dust particles may be associated with increasing heat release in a plasma with the dense dust structure [2] and the destruction of the plasma trap during the transition to the mode with the moving striations. Upon reaching such a low density of dust particles when the plasma losses on them are low, the electrical parameters of the plasma return to the initial state, the dust particles move to the center of the plasma trap and the process repeats.

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DUST CONCENTRATION INFLUENCE ON PLASMA CHARACTERISTICS OF THE DC GLOW DISCHARGE IN NEON

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The simulation was based on the drift-diffusion model of the uniform glow discharge positive column in neon with dust particles [1]. The losses of ions and electrons and quenching of metastable atoms on the surface of dust particles in a plasma bulk were considered [2]. The radial distributions of plasma components in a dust-free discharge and in presence of dust structures of various particles density are simulated. Dust particles cause additional losses of plasma particles on their surface and change the plasma ionization balance. The simulations have shown the changes of the radial profiles of plasma components at high concentration of dust particles. The increase of dust particle concentration leads to the case when the electron concentration on the outer face of dust cloud becomes higher than in the center of the tube, i.e. the maximum of electron profile shifts towards the tube wall, forming a local minimum in the center of discharge tube. When the dust particle concentration attains some critical value, the radial electric field changes its direction towards the discharge tube center within the dust structure. The simulations show the change in the radial distribution of electron concentration profiles caused by dust particles, resulting in the inversion of the radial electric field and causing the increase of the charge of dust particles in the vicinity of the border of the dust cloud at high concentration of dust particles. Dust particles loading in the glow discharge in neon is shown to lead to the noticeable increase of the longitudinal electric field strength. It is shown that the higher is gas pressure and discharge current the higher is the relative increment of the longitudinal electric field strength, caused by losses of plasma particles on the surface of dust particles. Within the dust structure, the metastable atom concentration was shown to be higher than in discharge without dust particles at the same discharge parameters.

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THE EVOLVEMENT IN SITU EXPLORATION THE PARAMETERS OF DUSTY PLASMA AT LUNAR SURFACE

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Theoretical insight about photoemission properties of lunar regolith interacted with solar flux is noted distinction by parameters from current investigations. The characteristic dusty plasma at lunar surface has some open questions where main of these is quantum yield of photoelectrons from regolith particles. The flux of Solar wind is supported effects of density distribution of dusty plasma particles and electric fields depend of altitude. In order to determine the effect of quantum yield of photoelectrons (within the context of exist uncertainty) there is provided direct experiment on lunar lander modules. The PmL instrument of Luna-Glob and Luna-Resource coming mission is allowed to realize measurements on Moon ground of the branches of energy spectra electrons and ions in lighted and shaded phases used in Longmire probe in range from −80 to +80 V. In addition the movement investigation of dusty plasma particles by sensitive piezo-ceramic sensors and electro-induction probes of PmL instrument are allowed getting in the evolution dusty plasma upon surface our closest space sputnik.

DUST STRUCTURES IN CRYOGENIC DC DISCHARGE: SOME SUGGESTIONS FOR FUTURE RESEARCH

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This paper discusses the current and potential use of cryogenic dc discharge in dusty plasma studies, with particular reference to experimental issues. Gas discharges at cryogenic temperature of atoms have many features that may occur in experiments with dusty plasmas. In particular, in dc low-pressure glow discharges at cryogenic temperature of discharge tube walls strong anisotropy of ion velocity distribution function takes place. This, in turn, can cause considerable change of the discharge dust structure properties. Experiments are conducted with micron-sized particles in dc glow discharge at gas temperatures of about 5-77 K. The results of recent numerical simulations and theoretical analysis of ion drift in depen-

dence on atom temperature are discussed. Tasks for future investigations are formulated.

STRUCTURE TRANSITIONS IN SMALL CLUSTERS WITH YUKAWA INTERACTION POTENTIAL

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The small systems of interacting particles are actively studied in various fields of science and technology, including nanoengineering and materials design. One of the most interesting and important questions about the properties of small systems is the exploration of their phase states and phase transitions. But the classical thermodynamical approach is inapplicable for this problem.

In this case, methods of analysis of dynamical systems appear to be very effective; in particular, the "dynamic entropy", the concept introduced by Shannon [1] and later developed by Kolmogorov and Sinai [2]. The value of the dynamic entropy decreases when the system orders, and its exploration of the phase space becomes more difficult [3]. In this work we use the simple approach for the estimation of the dynamic entropy, which can be easily applied for the analysis of the experiments and for the numerical simulation - so-called "mean first-passage time", MFPT entropy [4, 5].

In present work, the results of the numerical simulation of the dynamics of two-dimensional clusters of 7 and 18 particles interacting via the Yukawa potential are presented. The simulation was carried out by the Langevin molecular dynamics method; for the details see [6].

We have numerically obtained the MFPT entropy functions for the various values of kinetic temperature, corresponding to the conditions of the laboratory experiments with gas-discharge dusty plasma. Three phase states of the considered small systems are registered: crystal, liquid and transitional. The mechanism of phase transitions in the systems under study is described.

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RELAXATION TIME IN A MODEL OF DUSTY PLASMA

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The dusty plasma consists of solid particles and ionized gas. The particles diameter is several micrometers. Dust particles acquire a significant negative charge due to the different mobility of electrons and ions. The number of dust particles in laboratory experiments can be from one to thousands of dust particles. Dust particles can acquire kinetic energy of 10 eV and even more, which is much higher than the temperature of ions and electrons in gas discharge and the temperature of dust particles substance. The dust particles levitation is provided by the fact that gravity is compensated by the electric force. This force is conditioned by the influence of the electric field in the near-electrode layer on the charged dust particles. This is a core reason which leads to the asymmetry problem. Average kinetic energy of the dust particles vertical motion may differ significantly from the average kinetic energy of the horizontal motion of dust particles due to this asymmetry. The relaxation processes affect many aspects of dusty plasmas study. In particular, the determination of the system equilibrium and the determination of the systems which can attain equilibrium are directly linked to the issue of relaxation of all degrees of freedom of dusty plasma structures. The system equilibrium is the first requirement for the use of thermodynamic functions for the description of plasma-dust system. In particular, there is a question of equality of the average kinetic energy of dust particles and the term "temperature". In addition, the asymmetry of forces which influence dust particles motion leads to the specific mechanisms of energy transfer between the degrees of freedom and further complicates the determination of the relaxation mechanism and the relaxation time of the subsystems in dust particles system.

A method for the relaxation time estimation in nonideal dusty plasma is proposed. Estimations for the characteristic relaxation times of vertical and horizontal motion of dust particles in gas discharge are obtained.

These relaxation times appears to be different. The relaxation time of dust particles system moving in all three directions is also estimated. A single hierarchy of relaxation times is proposed. The applicability of the thermodynamic functions for the description of plasma-dust system is discussed.

EXTENDED MATHIEU EQUATION IN DUSTY PLASMA

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Phenomenon and mechanisms of an energy transfer between degrees of freedom of a dusty plasma system are of great interest in the field of dusty plasma. Since fluctuations of dust particles in the gas-discharge plasma on vertical and horizontal directions are largely independent, motions in this directions can be separated. So the dust particles motion and some of the energy transfer mechanisms can be described by the extended Methieu equation: $\ddot{x}+2\lambda\dot{x}+\omega_0^2(1+hcos\omega_p t)x=\eta(t)$, where $\eta(t)$ is a random force.

There are an approximate analytical solution for the Mathieu equation $\ddot{x}+2\lambda\dot{x}+\omega_0^2(1+hcos\omega_p t)x=0$ in the approximation of small h, $\varepsilon=\omega_p-2\omega_0/n$ and λ [2].

Acting by an analogy with [2] and using averaging over an ensemble of distributions of $\eta(t)$, we can obtain an expression for the growth rate of the amplitude s. The resonance areas boundaries obtained analytically and the ones obtained numerically are close only for nonfriction system with if $h<1$.

The approach proposed in [2] leads to serious differences with the numerical solution of the equation In the presence of friction ($\lambda\neq 0$). This is due to the fact that this approach takes into account only terms of zero-order of smallness with λ. The authors have proposed a solution that takes into account terms of other orders of smallness. The results obtained this way are closer to the data obtained numerically. It also explains such phenomenon as the shift of the ω_0/ω_p value wherein the resonance occurs with a minimum value of h.

The extended Mathieu equation is researched for a wide range of parameter values. Using analytical and numerical approaches derived boundaries of the resonance area, the time of onset and the growth rate of the amplitude at various system parameters. The results of the calculation are compared with various approximate analytical solution and the theory is specified in the places of disagreements.

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SOLUTION OF THE INVERSE LANGEVIN PROBLEM FOR OPEN DISSIPATIVE SYSTEMS WITH ANISOTROPIC INTERPARTICLE INTERACTION

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It is well known that a charged particle or macroobject, immersed in a flowing plasma, creates a perturbed region (a wake) behind itself. Wakefield potential is often invoked to explain a vertical alignment of dust particles levitating in the plasma sheath of capacitive radio-frequency (RF) discharge. In such a plasma ions have a directed velocity relative to stationary dust particles which can lead to focusing of ion fluxes behind negatively charged particles and, as a consequence, to difference between the interaction of dust particles in the directions perpendicular to the ion flow and parallel to it.

To date, the experimental determination of the pair interaction forces have been carried out between horizontally aligned particles [1], [2] suspended in the sheath of capacitive RF discharge; as well as between heavy probe particle and dust cloud in the diffuse edge of inductive (electrodeless) RF discharge [3]. In all this cases the interparticle interaction can be described in the isotropic approximation.

In this report we consider a possibility of experimental diagnostics of anisotropic interaction forces between dust particles in plasmas, arising due to effects of ion focusing. To recover anisotropic interparticle interaction forces we improved the method based on solving the inverse Langevin problem [2].

We verified the method on the results of numerical simulation of chain structures of particles with quasidipole-dipole interaction, similar to the one occurring due to effects of ion focusing in gas discharges. It was shown that the proposed method can recover the spatial distribution of anisotropic interparticle interaction forces, and can be used for diagnostics of a laboratory dusty plasma with ion flow. An influence of charge spatial inhomogeneity and fluctuations on the results of recovery is also discussed.

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THE EFFECT OF NONRECIPROCAL INTERACTION ON THE REDISTRIBUTION OF KINETIC ENERGY IN THE SYSTEM OF PARTICLES

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Under certain conditions (e.g., pressure changes, or increase of the particles number) of particles of dust in the laboratory plasma can acquire kinetic energy stochastic ∼5.1 eV, which is higher than the temperature namnogoi surrounding gas. A distinctive feature of the observed structures is dust temperature increase in the direction of the ion flow (from the upper layers to the lower layers of multilayer particle structures), and also the possible difference in the distribution of particles kinetic energy in the degrees of freedom (in the direction of ion flow the kinetic energy of the particles is often higher than its radial component). The basic mechanisms for the growth of kinetic energy of the dust particles are usually associated with different temporal and spatial changes in their charges [1]. The behavior of dust particles with anisotropic interaction could significantly differ from the isotropic case. For example, in multilayer dust crystals, anisotropic interaction of dust particles could cause vertical string-like alignment of adjacent layers. During the numerical simulation of particle systems with the anisotropic nonreciprocal pair interaction we observed an anomalous rise in stochastic kinetic energy of dust particles [2, 3]. We here consider the features of redistribution and growth of kinetic energy in the particle system with nonreciprocal interaction. Numerical and theoretical studies carried out for two vertically arranged particles with anisotropic interaction, similar interaction occurring due to effects of ion focusing in the conditions of experiments with laboratory dusty plasma. The proposed analytical expressions are suitable for the analysis of the dynamics for systems with different nonreciprocal interactions such as gyroscopic forces, inertia forces in inertial and non-inertial systems, etc.

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ANALYSIS OF THE PHASE STATE OF SMALL-SIZED MONOLAYER DUSTY PLASMA SYSTEMS USING GLOBAL ORIENTATIONAL ORDER PARAMETER

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To study the melting processes in monolayer dusty plasma structures standard methods are typically used, such as analysis of the shape of pair and bond-angular correlation functions, which has strict limitations on the number of observed particles and the degree of uniformity of the studied systems. Often in laboratory experiments with dusty plasma, the formation of various irregularities, in particular the so-called domains, is observed, which can significantly affect the melting process in the two-dimensional non-ideal structures. In this regard, the study of global order parameters (translational and orientational) seems promising, since these parameters will vary appreciably even in the real experiments with dusty plasma structures with different structural pertubations, and they are suitable not only for extended monolayer structures, but also for systems with a small number of particles. In our work we present the results of a numerical and experimental study of the global orientational order parameter as a function of coupling parameter of two-dimensional system, as well as of the number of particles in the small-sized (cluster) systems. The calculations were performed for non-ideal two-dimensional system of particles interacting via Yukawa potential in a wide range of parameters corresponding to the experimental conditions in the laboratory dusty plasmas. The global orientational order parameter measured from experiments with monolayer dusty plasma structures of small sizes, formed in the near electrode area of RF gas discharge, was also analyzed.

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ON MELTING DENSITY GAP AND NON-CONGRUENCE OF PHASE TRANSITIONS IN MODELS OF DUSTY AND COLLOID PLASMAS

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Two simplified variants of dusty, CDP (condenced dispersed phase) and colloid plasmas models are considered as a thermodynamically equilibrium combination of classical Coulomb particles: a 2-component electroneutral system of macro- and microions (+Z,-1) and a 3-component electroneutral mixture of macroions and two kinds of microions (+Z,-1,+1). The base for a consideration is the well-known phase diagram of dusty plasma [1] for an equilibrium charged system with the Yukawa potential in its standard representation in the coordinates: Γ - κ (Γ is the Coulomb non-ideality parameter, κ is the dimensionless Debye screening parameter). The phase regions for the three states of the system (fluid vs. bcc and fcc crystals) from the phase diagram [1] are reconstructed in the density-temperature coordinates. The resulting phase diagram in the logarithmic coordinates has the form of a linear combination of crystalline and fluid zones separated by the boundaries Γ = const. Parameters and locations of these zones are analyzed in dependence on the intrinsic parameter of the model - macroion charge number Z. Parameters of a splitting the one-dimentional melting boundaries of the Hamaguchi diagram (i.e. hypothetical melting density gap between separate freezing liquid line (liquidus) and melting crystal line (solidus)) are discussed. Made an estimation of a density gap value based on an analogy with a Soft Sphere system model and a Hard Sphere system model. Additional splitting of all phase boundaries in the three-component model (+Z,-1,+1) because of so-called non-congruency of all phase transitions in this model is discussed also.

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H_α LINE DOPPLER BROADENING IN A GLOW DISCHARGE CATHODE REGION IN THE ARGON–HYDROGEN MIXTURE

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Spectral measurements of Doppler profiles of the hydrogen H_α line in glow DC discharge in a mixture of hydrogen and argon (1% of hydrogen) at pressures of 60, 120 and 180 Pa were performed. Solid and mesh cathodes were used. It is brought out that the width of the line corresponding to the effective temperature of the excited atoms of 40 ± 7 eV, does not change when the pressure and the distance from the cathode in the region of negative glowing and increases slightly with distance from the mesh cathode outside of the discharge gap.

INFLUENCE OF COLD ATMOSPHERIC PLASMA TREATMENT ON BACTERIAL AND EUKARYOTIC CELLS

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In our work we present the results of an experimental study of the effect of non-isothermal low-temperature microwave argon plasma under atmospheric pressure, generated by the developed medical plasmatron, on bacterial and eukaryotic cells at various regimes of plasma generation. We obtained the modes of plasma generation (including exposure, the gas flow rate, the electrode gap and the distance to the cells treated in vitro), at which a pronounced bactericidal effect in the absence of toxic effects on human eukaryotic cells was achieved.

To study the bactericidal effect of argon microwave plasma generated by a modified power source, we used microorganisms most frequently contaminating the wound surfaces: Gram-positive Staphylococcus aureus ATCC 25923 and Gram-negative Pseudomonas aeruginosa Pa103 which have a multiple antibiotic resistance. As a result, it was found that the Gram positive S.aureus was more resistant to the effects of plasma and Gram-negative P.aeruginosa showed greater sensitivity. To determine the possible toxic effects of low-temperature plasma (LTP) for eukaryotic cells

we used cell types that form the wound surface and participating in the closure of wound defects: a cell line of human fetal lung fibroblasts with properties similar to dermal fibroblasts, and immortalized human keratinocytes HaCaT. The study cytotoxicity we used xCELLigence (Roche) system, allowing tracking the rate of proliferation and cell death in real time in 96-well plates. To study the possible toxic effects of LTP we chose modes, which showed the greatest efficiency in experiments with pathogens. It has been found that plasma treatment in these conditions did not have a toxic effect, and in 120 hours after plasma exposure cell death was not observed.

Thus it is shown that the low-temperature plasma generated by the developed power source can have a strong bactericidal effect against multi-antibiotic resistant microorganisms, and be non-toxic to the eukaryotic cells at the same time.

NONLINEAR DIFFUSION WAVE IN THE HIGH MAGNETIC FIELDS

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The processes of nonlinear diffusion of the magnetic field into a conductor and a plasma formation on the surface of a conductor in fast rising strong magnetic fields are very important for the efficiency of electromagnetic energy transport by the vacuum transmission line of pulsed power generators with a current amplitude of 50 MA and a rise time of 100–200 ns.

EXPERIMENTAL STUDY OF THE X-PINCH HOT SPOT STRUCTURE WITH SUBNANOSECOND TEMPORAL RESOLUTION

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Two or more metal wires 10-50 microns in diameter crossed like the letter X are used as the X-pinch loads for pulsed power generators. When an X pinch is powered by current pulse a so called plasma hot spot several

micrometers in size can be produced. This hot spot radiates soft x-rays in a 1-2 ns pulse. X-pinch-based soft x-ray sources are attractive for backlighting projection imaging of various short-living physical objects. As a rule a simple point projection scheme is used in such experiments. A sample under investigation is placed between the X-pinch and photographic film. Due to low hot spot size spatial resolution order of few microns can be realized, while short radiation pulse provides nanosecond temporal resolution. Backlighting images produced with an X-pinch are often featured by smashing or doubling of the sample shadow. That means that hot point has a complicated internal structure. In order to investigate hot point plasma behavior a soft x-ray streak camera AXIS-NX was used with a picosecond temporal resolution. X-pinch experiments have been performed on a compact 250 kA, 180 ns pulsed power generator fabricated at the Institute of High Current Electronics (Tomsk, Russia). The X pinches were composed of two or four molybdenum wires of diameter 25 microns. Backlighting images of a static sample (tungsten wire) with a temporal resolution of 20 ps were registered. It was shown that in the spectral range 1 -1.55 keV the hot point consisted of a few radiation sources which could be shifted from the X-pinch axis by 10 microns approximately. Each source generated radiation pulse with duration of 0.2-0.7 ns. The time interval between these x-ray pulses was measured to be 0.5 ns or higher. Possibly a fine adjustment of the X-pinch initial parameters would allow avoiding of the multiple sources forming.

STRATA FORMATION DURING THE FOIL EXPLOSION IN VACUUM

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The formation of the strata during fast explosion of metal foils at current densities of 100 MA/cm^2 has been studied experimentally. To observe the strata the soft x-ray radiation generated by an x-pinch were used. The experiment on studying the process of stratification during the foil explosion (FE) was carried out in a setup consisting of three generators. One of generators (WEG-2) was operated to initiate FEs, while the others (XPG radiographs) were used for diagnostics. The generator WEG-2 has the capacitance of 250 nF, the charge voltage of 20 kV, and the current rate of

16 A/ns. The radiographs XPG have the capacitance of 1 μF, the charge voltage of 43 kV, the current of 300 kA, and the current rise time of 180 ns. X-pinch produced by four Mo wires was a load for the radiographs. The delay between the operation of the WEG-2 and XPG generators was set with the use of DPG trigger pulse generator; the operation jitter was 20 ns for the all generators. The delay between the operations was regulated in the range from 0 to 1.3 μs. We performed the experiments with the Al and Cu foils. The length of foil was 2 cm, the foil width was 1 mm, and the foil thickness was 6 μm. In our experiments the shunting discharge develops at the metal explosion in the vacuum. It has been revealed that strata were formed early in the explosion, i.e. at the stage where the metal melted. Analysis of the experimental results suggests that the most probable reason for the stratification is the thermal instability developing as a consequence of the increase in resistivity of the foil metal with temperature.

INVERSE PROBLEM OF THE CURRENT PULSE RECONSTRUCTION ACCORDING TO THE PENETRATION RATE OF ELECTRIC FIELD INDUCED INSIDE THE TUBULAR ELECTRODE

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A series of numerical simulations was carried out to study the evolution of hollow tube matter during exposition by submicrosecond current pulse with linear density of 1–3 MA/cm. The experiments with the same linear density were conducted on the Angara-5-1 installation. In this way the behavior of the electrodes under extreme energy and strength loads was simulated in those experiments and calculations. To obtain reliable results, the experimental time dependence of the current ought to be specified as boundary conditions during all time the process is modeled. However, the reliable current measurement was carried out within the first ∼100 ns in these experiments. The evolution of tube material is of interest for a longer time period. To solve this problem the time dependence of current ought to be restored according to the time dependence of the electric field intensity, measured on the inner tube surface during 500 ns. For this purpose the inverse problem was solved; the data obtained were used in the MHD-simulation.

HIGH-CURRENT CHANNEL STRUCTURE AT HIGH DENSITY GAS

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Research results for discharge, initiated by wire explosion, in hydrogen at initial pressures of 1–200 MPa and current amplitudes up to 1.5 MA are presented.

The discharge has very complex channel structure. Narrow axial zone with high temperature generate x-ray radiation flux. Transient photoionized plasma zone between current channel and surrounding gas produced by the flux. Surrounding gas decrease energy losses from discharge channel, assisting channel plasma overheating. Acoustic oscillations in discharge volume and channel radius oscillations produce x-ray radiation modulation by convergence of acoustic compression wave on discharge axis.

Two types of channel oscillations in super-high pressure discharges are registered [1]. The first oscillation type, in our opinion, is connected with the alignment of the magnetic and gas-kinetic pressures in the discharge channel. The second one is connected with acoustic oscillations in a whole volume of the discharge chamber. It is shown that oscillations of first type produce x-ray radiation modulation. Similar phenomena had been shown in fast discharges, where x-ray intensity modulation were explained by convergence of acoustic compression wave on discharge axis [2].

Measurements of channel radius oscillation amplitude by magnetic probe diagnostics were maid for calculation of x-ray oscillation intensity. Oscillation amplitude was decreased with initial gas pressure grows and increased with current amplitude rise. This phenomenon and, also, increasing oscillation amplitude with grow of plasma atom number give a suggestion that first type oscillations were connected with changing of radiative characteristics of discharge channel, similarly as in [3].

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PARAMETERS OF ELECTRICAL DISCHARGES WITH LIQUID METAL ELECTRODE

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The work is devoted to investigation of parameters of high current electrical discharges forming under free surface of liquid metal in tasks of melting and mixing intensification with use of electrovortex flow control [2, 3]. The significance of the investigations is to solve fundamental [1] and application problems related to improving the performance of technical devices for increasing of efficiency in power engineering and industry, as well as related to improving the environmental situation. One of the applications of research results is metallurgy. Systems with electric arcs under liquid metal surface taking place in many electrometallurgical processes: electroarc melting, re-melting, casting, welding, getting of liquid metal heat transfer agent, melt purification, getting aluminum in electrolyzers, waste recycling. Measurements of electrical, thermodynamic, spectroscopic and magnetic characteristics, visualization of formation, evolution and structure of the high-current arc in the following conditions: pressure - 1 atm, ambient gas - air, nitrogen, electric current values - from 1 to 30kA, liquid electrode - lead, tin, eutectic alloy of indium-gallium-tin, will be carried out. The electric arc will be initiated in the electrode gap of a rode electrode of various diameters and a bath of melt of model metal (lead, tin, indium-gallium-tin). Special heaters will provade formation of the bath of molten model metal. Capacitor banks of following parameters: voltage - 50kV, power - 100kJ, duration of a current pulse - up to 100mks and 10kV, 6MJ, up to 3ms, will be used as an energy source for electrical discharge burning. With the use of high-speed optical techniques it is supposed to to carry out comprehensive diagnosis of the formation and evolution of the electric arc and to determine parameters of the arc channel. High-speed photorecording will allow visualizing a liquid metal constriction formating inbetween the electrode and the liquid metal, electrical explosion of the constriction and subsequent ignition of the discharge. Temperature of the plasma channel will be determined from the spectral measurements, and temperature of molten metal surface in vicinity of the arc will be determined by high-speed pyrometer. The work is supported by RFBR N 14-08-31078.

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SPARK FORMATION IN THE SAND AT PULSE SPREADING OF CURRENT

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Process of spark formation in laboratory experiments on pulse current spreading from rod and angular electrodes was investigated. Process of sparking was fixed by means of video filming of electrodes through a special lateral window which was approached to electrodes. When the rod electrode with sphere at the end is utilized formation of plasma channels is observed at the voltages above eighteen kilovolt. The passage of high current causes a significant medium heating, gas-dynamic expansion of the channels, and finally shock-wave formation. Sand expulsion from the cylinder and formation of two cantimeters width cavity were observed under the one second kiloampere current pulse. Spark formation at the angle bar electrode is the most intensive in the areas of field enhancement where current density is higher. Pictures of the spark channels are distinguish at different water contents. At low humidity of the sand plasma area has a torch-like shape while at the high humidity the long spark channels develops. It is interesting to note that the glowing near the electrode has a ten times greater duration than the voltage pulse has.

FORMATION OF OVERHEATING INSTABILITY IN NON-LINEAR CURRENT SPREADING IN THE SAND

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Laboratory experiments on pulse current spreading from spherical electrodes and evolution of electrical breakdown of silica sand with different water contents under 15–20 kV pulse voltage have been performed.

It is shown, that dramatic nonlinear decrease in pulse resistance of soil occurs when current density exceed a certain threshold value. Then ionization-overheating instability develops and leads to current contraction and plasma channels formation in soil. The method for determination of threshold electric field for ionization is proposed. It was found that electrical discharge in wet sand develops with significant delay time for long discharge gaps similar to thermal breakdown.

CONFINING BOUNDARY CONDITIONS FOR SIMULATION OF INTERACTING FERMIONS BY ANTISYMMETRIZED WAVE PACKET MOLECULAR DYNAMICS

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The method of Wave Packet Molecular dynamics [1] is an approximate quantum method for numerical simulation of many-particle dynamics. In this method single electron wave functions are expanded in a set [2] of floating Gaussian wave packets (WP) φ_k. A trial many-body wave function is constructed depending on the quantum statistical properties of the simulated ensemble, for example for fermions (electrons) a single Slater determinant antisymmetrized product is usually used for each spin projection. The resulting equations of motion follow from the variational principle [3].

In this work we study a system of electrons in a 3D confinement potential constructed from harmonic walls and a flat floor in each spatial direction. The matrix elements of the proposed potential with Gaussians were obtained analytically. The confined system constructed this way is an excellent testing ground for AWPMD method, because it poses correct quantum boundary conditions; reduces to textbook many-body quantum oscillator in the limit of no interaction; reduces to uniform quantum gas when the floor size is large.

The unlimited broadening of the Gaussian wave packets and underestimation of the electron-electron and electron-ion collision frequencies is known to be the major problems of the WPMD method [4] when applied to many-particle systems with homogeneous density, for example plasma systems. We show however that the method is able to excellently describe the thermodynamics of a confined fermionic system. The infinite WP broadening is directly related to the infinite statistical sum in an unconstrained

system and does not appear in the confined system. For example, the nearest image boundary conditions guarantee the periodicity of expectation values but do not limit the number of allowed states in the simulated system.

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DYNAMICS OF ELECTRONS IN LASER PRODUCED CLUSTER NANOPLASMA

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The nanoplasma produced by laser pulses of moderate intensities (10^{13}–10^{16} W/cm^2) targeted at metal clusters is studied by molecular dynamics (MD) simulations. Whereas a lot of the cluster plasma studies are concerned with the Coulomb explosion of the ion core we focus on the electron dynamics just after cluster ionization. In particular we consider electron eigenmodes and electron emission depending on the cluster size and plasma temperature.

One of the distinguishing features of the cluster plasma 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. With respect to a small number of particles in the clusters under consideration (10–10^6) this charge determines the rate of plasma expansions, affects the rate of ionization-recombination processes, electron density profile, and optical properties of the cluster plasma [1–3].

In this work we propose a model of thermionic emission of nanoclusters based on our MD simulation results [6]. This model qualitatively explains known experimental results [5] and it is in a good agreement with other simulations [4]. The dependency of the electron oscillation spectrum on the cluster charge is discussed. The frequencies and damping rates of different electron eigenmodes including Mie and Langmuir oscillations are obtained.

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ION SOLVATION AT DIFFUSION IN SIMPLE LIQUIDS

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A research of the diffusion of an ion in a liquid is carried out. Dependences of the diffusion coefficient on the ion-molecule potential, ion mass, liquid temperature and density are defined. The results are related to the ion solvation. The classical molecular dynamics method is applied.

The polarization potential $U(r) = \beta/r^{12} - \alpha/r^4$ is used to describe the interaction of the ion with molecules of the liquid. The Lennard-Jones potential $U(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6]$ is used to describe the intermolecular interactions. The model can be reduced to 5 parameters parameters: α, β, ion mass, liquid temperature and density, whereas σ is the unit of length, ε is the unit of energy and liquid molecule mass is the unit of mass. The wide range of different ions and liquids at different thermodynamic conditions are investigated.

The effect of the ion solvation is discovered. A rather weak dependence of the diffusion coefficient on the ion mass is the first argument. This is due to the fact that the total mass of the cluster formed by the ion and the ion solvation shell varies slightly while the mass of the ion changes significantly. Also, the dependence on β is found to be rather weak. This is because β defines mostly the geometry of the cluster, whereas the polarization part of the ion-molecule potential influences the interaction of the cluster with the ion environment. The dependence of the diffusion coefficient on α is found to be really stronger than on β. The ion velocity autocorrelation function calculated reveals a strong oscillatory character superimposed on the conventional functional liquid-type form. It reflects the oscillations of the ion inside the solvation shell. The lifetimes of the cluster molecules are estimated as a function of the ion-molecule distance.

The dependence of the ion mobility on temperature is found to be of the Arrhenius-type form. The dependencies of the ion mobility and diffusion on the liquid density are close to linear.

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THE INFLUENCE OF PLASMA ACTUATORS MATERIAL AND GEOMETRY ON THE ELECTROMAGNETIC CHARACTERISTICS OF THE DISCHARGE AND THE SPECIFIC THRUST OF SYNTHETIC JETS

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There has been a number of studies on the properties of wall jets produced by the dielectric barrier discharge of plasma actuators. There were many variations of electrodynamic [1] and geometric parameters of actuators [2, 3].

There was the question: how material of the electrodes influence on the process [4]? Formating of the synthetc jet begins from releasing of electrons from the exposed electrode. That's why ionisation energy of material of electode strongly influences on the ionization degree of the ambient air. Material with lesser ionisation energy emitting more electrones per sec. It leeds to rising of the force that acts on the stream. Thereby the output of synthetic jet is rising. The role of the specific resistance is ambiguous. Its increasing to a certain value contributes to rising of specific thrust at its extreme value relative to the distance between exposed electrodes. With further increasing it was shown inverse effect which was especially noticeable when we used electrodes of non-linear shape.

In this paper, we examine the effect of the electrode material on the value of specific thrust of the synthetic jet produced by symmetric actuator. The dependences of specific thrust on the distance between external electrodes for copper, aluminum, nickel, and titanium was made. A considerable effect of the shape of the external electrodes on the electric field and current density in the tape drive, and the specific thrust of the synthetic jet was investigated. It was also evaluated the role of autoelectronic emission on the current in streamers and the value of volume force acting on the stream.

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CREATION OF THE EXPERIMENTAL SETUP WITH A PEAK CURRENT UP TO 400 kA IN SUBMILLISECOND RANGE TO OBTAIN LONG-LIVED PLASMA CLOTS

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To obtain long-lived plasma clots previously we used a toroidal installed multiturn electrically exploding copper spirals that at the time of electric explosion has created an impulse of toroidal magnetic field with amplitude at the level of 2 Tesla. Electric explosion of spirals was carried out using the experimental setup of 'INGIR-Mega-15', which allowed obtaining the peak current level of 35 kA with pulse duration of 0.5 milliseconds. Submillisecond range of pulse durations were used in order to allow for effective penetration of current inside fairly thick copper conductors. The aim of this work was to obtain long-lived plasma clots with a lifetime of at least 3 seconds. To date, however, in the experiments, the lifetime of plasma clots (the best result) did not exceed 1.6 seconds. The reason was that used multiturn helix peak current expressed in ampere-turns, rarely reached 200 kA, and its increase was not possible due to premature breakage of the spirals. Therefore, it was decided to use single-turn spiral or linear inductors, which are less critical to premature breakage of conductors. According to theoretical estimates, to obtain plasma clots with a lifetime in the order of 10 seconds, it is necessary that the peak current was of the order 400 kA. It has been the aim of the ongoing upgrade of 'INGIR-Mega-15'. To do this, the capacity of the capacitor Bank was increased from 0.25 to 1.12 F at a voltage of 450 V and strengthened the switch current: thyristors instead of 10 was used 112 thyristors type TB261-160-12 with peak currents up to 4 kA in each of them. The internal resistance of discharge circuit of the experimental setup is no more than is 0.0002 Ohms. In preliminary experiments, we used two copper wires with a diameter of 1.2 mm and a length of 15 cm that were electrically connected in parallel. The amplitude of the discharge current in the electric explosion in this case amounted to about 50 kA. In the future, we plan to use 16 such wires, and according to a rough estimate, it should provide the peak value of the pulse current at

400 kA. As a result, we hope to get a plasma clot with a lifetime of more than 3 seconds. This work was supported by the Ministry of education and science of Russia, the contract 14.518.11.7002 dated 19 July 2012.

EVOLUTION OF DISCHARGE CHANNEL IN IPA SOLUTION

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Discharges in liquids are used in various fields of human activity, such as medicine (extracorporeal shock wave lithotripsy), construction (electrohydraulic machine and reuse of construction materials), and ecology (eliminating bacterial, organic and inorganic impurities). Many researches have been done on discharges in liquids with variety of electrode sets. In this paper we report observation of the pulse discharge channel propagation after its initiation in 15% IPA solution.

In our experiment, stainless still (anode) and copper (cathode) electrodes are placed in the vertically oriented 16.6-mm inner diameter quartz tube with anode electrode at the top. The anode tip has a conical shape with apex angle of 20°C and cone basis diameter of 3 mm. The cathode tip has a hemisphere shape with radius of 1 mm. The electrode gap is 15 mm. High voltage pulse voltage generator (HVPVG) with inner storage capacitor of 1.6 mcF and (0-40) kV output voltage is used for spark generation. Half amplitude pulse duration is about 10 ms. Ballast resistance limits current value less than 3A. Voltage and current across the discharge gap are measured by Tektronix DPO7054C with high voltage probe and current shunt respectively. The applied voltage pulse has positive polarity. The discharge is synchronized with the CMOS RedLake MotioPro X3 camera. The results of the experiment revealed the following phenomena. The anode region glowing appears in (500-600) mcs after voltage applying due to ionization-overheating instability near the surface of anode electrode. Obtained images show channel developing from this region. Partial discharges are observed in the near region along the whole length of the channel during its evolution. These discharges most likely occur in gas bubbles. Their formation due to vaporization during the Joule heating of highly volatile fraction with conduction currents was observed in subsidiary experiment without electrical breakdown of the electrode gap. Bubble breakdown in front of channel tip was observed. The channel reaches cathode in 4 ms

after the anode glowing appearance. The propagation velocity is about 4 m/s. After the gap is bridged the discharge channel heats up and intensive cathode glowing appears. The most of energy deposits in the cathode region. The destruction of spark channel takes about 2 ms. After the discharge current drops anode glowing almost disappears opposite to cathode glowing with additional (4-5) ms life-time.

RADIATIONS AND STRUCTURE OF HIGH-VOLTAGE ATMOSPHERIC DISCHARGE

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Recent studies of natural lightnings show that the high-energy radiations are generated during thunderstorms. Besides hard x-ray and gamma radiation, a neutron generation is also observed. In a laboratory long spark discharge with the parameters similar to lightning such phenomena are observed also. Experimental results on registration of different types of radiation (RF, optical, UV, X-rays and neutron) are created at initial (dark) phase of high-voltage atmospheric discharge (before the streamer-leader stage) are presented. The model to explain the generation of hard x-rays and neutron bursts during atmospheric discharge in air is under discussion.

Experiments with the formation of 500-700 mm long sparks in air were carried out on ERG installation (LPI, 1 MV, 60 kJ, 150 ns risetime) at different initial electric field distributions. A volumetric streamer corona of 0.2-1.0 kA on both of electrodes at atmospheric pressure was followed by a formation of bright channel of 12 kA leader. Time-resolved UV and X-ray radiations were registered by pulsed FM-tubes of different types integrated with scintillation detectors. The registration of neutron emission in the real-time mode was performed by plastic scintillation detectors placed inside Pb shield. Neutron emission occurs at the very beginning of the discharge and correlated with X-ray radiation: neutron pulse always was placed inside X-ray one. Hard X-ray pulse is followed by neutron pulse very seldom. An anisotropy of hard radiation was observed. It could indicate a presence of collective mechanisms of particle acceleration. A fine microstructure of a leader stage of a 200-1200 ns discharge was observed. The distribution of micron-scale microchannels over the mm-size leader cross section near the electrodes and in the gap was investigated. Optical and autograph diagnostics were used to estimate a current density in a

single microchannel. The possibility of current carrying by the relativistic electrons drifting in the crossed electric and magnetic fields and the acceleration of ions to keV energy range in a strong radial electric field at experimental conditions was examined. The observed experimental results are compared with the filament model estimations of x-ray emission intensity and neutron flux.

The work is supported by RFBR Grants 13-08-01379, 14-08-31397.

THE RUNAWAY ELECTRON BEAM FORMED IN A DISCHARGE AT ATMOSPHERIC PRESSURE

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A numerical model is proposed which allows one to describe the dynamics of the fast electrons injected from the head of an anode-directed streamer. The model is based on solving numerically equations of motion of electrons. In the context of the model, the number of electrons which can be injected from the surface of a streamer is determined by the number of electrons in the Debye layer.

SYNTHESIS OF GRAPHENE MATERIALS BY PYROLYSIS OF HYDROCARBONS IN THERMAL PLASMA AND THEIR PROPERTIES

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Perspective materials for supercapacitor electrodes are carbon materials produced from natural renewable raw materials. Their specific surface allows to store large amounts of energy in the electric double layer, and the availability of raw materials makes them attractive from an economic point of view. From this point of view it is of interest to obtain and investigate graphene structures containing two or more (up to 10) with a slit-pore layers.

For the synthesis of graphene materials thermal plasma generator was used which is a high current divergent anode-channel DC plasma torch. The experiment involved the simultaneous input of hydrocarbons (methane, propane, butane, acetylene) with the working gas (helium, argon) into the plasma torch, and wherein the heating and the pyrolysis occurred in the plasma jet and in the region of the arc discharge, followed the condensation of product of synthesis on metallic surfaces. The consumption of carbon, the plasma forming gas and the plasma torch power were changed independently from each other. The resulting products have been investigated by electron microscopy, porosimetry, thermogravimetry and X-ray diffraction.

Investigation has confirmed the formation of graphene materials. It was found that depending on the synthesis parameters changing geometry graphene materials (from curved petals to disk diameter of 400 nm - 1 mm) and graphene content in products of synthesis. To determine the characteristics of the porous structure (pore volume, pore radius, surface area) we have used a relatively new method of adsorption "Limited Evaporation" based on the analysis of the kinetics of evaporation of the adsorbate from the test material, and classical BET method using a low-temperature nitrogen adsorption - to estimate the specific surface of materials. It was concluded that the curves of pore size distribution corresponded to typical mesoporous samples with the main pore size in the range of 10 to 40 nm, and macropores were founded having a pore size of more than 60 nm.

The optimal conditions for the synthesis of graphene materials and the influence of synthesis parameters on the structure of the surface and specific pore area have been found.

THE STUDY OF ELECTRON IMPACT IONIZATION PROCESSES OF SUBSTANCE, WHICH SIMULATE THE COMPONENTS OF A SPENT NUCLEAR FUEL

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One of the priorities of nuclear power industry is the reprocessing of spent nuclear fuel (SNF). A new method of reprocessing of spent nuclear fuel is being developed in JIHT RAS nowadays. This method is based on a plasma separation technology and is alternative to common chemical methods [1].

It is necessary to study the ionization processes of a model substance, for the creation of a plasma source which is necessary for working off the plasma separation method (lead was chosen for modeling heavy SNF components). Lead has a sufficiently high atomic weight (207.2), which allows to carry out pilot experiments in which dynamic and kinetic properties of the heavy SNF component must be modeled.

The discharge in the lead vapors with density from n_a=10^{12} cm^{-3} to n_a=10^{13} cm^{-3} was analyzed numerically and analytically in a computational model. In the model the lead vapors (with a temperature of $T_a \sim$ 0.1eV) was injected into the space between two planar electrodes (the distance between electrodes is 10mm and the potential difference between them is up to 500 V). One of the electrodes was the heated emitter of the electrons. As obtained data shows, the single ionization efficiency (η) was significantly higher at the concentration value of $6 \cdot 10^{12}$ cm^{-3} than at the concentration of $1 \cdot 10^{12}$ cm^{-3} and reached the maximum (η=0,8%) in the boundary regime between the ion and electron brunches. The experimental module was designed and constructed. Its characteristics were close to the parameters considered in the computational model. Substance evaporation was carried out by crucible heating then lead vapors were injected into interelectrode space. The ion current of lead up to 400μA was obtained. Thus, the amount of the consumed energy didn't exceed 200 W. Experimental results were in good agreement with the computational model.

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GENERATION OF A CONTROLLED ELECTRIC POTENTIAL PROFILE IN THE MAGNETIZED PLASMA TO DEVELOP A METHOD FOR PLASMA SEPARATION OF SPENT NUCLEAR FUEL

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One of the key problems in the developing a method of plasma separation of spent nuclear fuel is the creation controlled potential profile in the plasma. To solve this problem it is necessary to create a buffer of a magnetized plasma and to develop a system of electrodes that define it the plasma a non-uniform electric potential. Plasma parameters of the buffer must satisfy the following requirements: the plasma density up to 10^{13} cm^{-3}, the volume of the working chamber of the plasma separator—about 1 m^3, with a magnetic field up to 2 kG. In view of these requirements a helicon plasma source is selected as the most promising. Based on the executed evaluations two different configurations of antennas were selected: coil and saddle types. In the experiments radial distribution of plasma density and electron temperature were obtained. Estimation of expected values was based on the works of Chen F. [1]. Non-uniform electric potential will be set by a system of electrodes located on the end flanges. In order to develop mechanisms of creating a non-uniform electric potential in the plasma discharge with different configurations defining electrodes was studied experimentally. The following electrodes were used: a ring configuration, a ring configuration with a central electrode, a configuration in the form of parallel strips. The study revealed the existence of two forms of discharge—"low-current" and "high-current". It was found that at a gas(helium) pressure of 1 mTorr current-voltage characteristics of a discharge had a monotonous character, and at a pressure of 35 mTorr CVC had non-monotonic character. Reproducibility of potential defining electrodes was shown in the volume of the separator in the presence of sufficiently high setpoint (1 kV). It was noted that the shape of electrodes affects the amount of reproducible potential, and the potential is less than the values given by the electrodes in 2–5 times for different geometries. The research was done by a grant from the Russian Scientific Fund (project No. 14-29-00231).

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THE STATIONARY VACUUM ARC ON NON-THERMIONIC HOT CATHODE

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Results of experimental study of vacuum arc with diffusive spot on plumbum cathode at temperatures 1.25–1.45 kK are presented. At these conditions current density of thermionic emission from cathode was less than 1 μA/cm^2, while the mean current density on the cathode was in the range 10–30 A/cm^2. Experiments were carried on vacuum chamber at residual pressure less than 10 mPa. Plumbum with mass of 15 g was placed in heat-insulated crucible (cathode) with external diameter 25 mm. Electron-beam heater was situated under the crucible. This heater could change the crucible temperature at the fixed current of arc. The water-cooled steel disc with central hole 15 mm in diameter was used as the anode. At the temperature of 1.25 kK which corresponds to plumbum saturated vapor pressure about 0.1 kPa voltage from power source (380 V, 200 A) was applied to anode, and vacuum arc was initiated. Arc current was changed in the range 20–70 A, arc voltage was about 15 V. Sometimes low-current discharge with current about 10 mA and voltage of 350 V has preceded arc ignition. After a few seconds this discharge has transformed in arc. The studied arc discharge is characterized by the absence of the random voltage fluctuations; the micro particles of cathode erosion products were observed only in transition regimes. Spectral data of plasma radiation and values of the heat flux from plasma to cathode were obtained. It has been experimentally established that the evaporation rate in arc approximately two times less than without discharge. Ionization degree of plumbum vapor in the cathode jet was in range 20–30%. Comparison of the characteristics of studied discharge on thermionic cathode from gadolinium and non-thermionic plumbum cathode was fulfilled. One can assume that the ion flow provides the charge transfer on the cathode surface in the studied discharge. The study was supported by grant from the Russian Scientific Fund (project #14-29-00231).

HIGH-VOLTAGE DISCHARGE IN SUPERSONIC JET OF PLUMBUM VAPOR

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During the investigation of vacuum discharge in plumbum evaporating from molybdenum crucible in identical geometry of discharge gap and the same crucible temperature existence of two different discharge forms were observed. These two forms are vacuum arc with current more than 10 A and discharge voltage about 15 V and high-voltage discharge with current of about 10 mA and voltage of 350 V.

Experiments were carried on vacuum chamber with residual pressure less than 10 mPa. Plumbum was placed in heat-isolated crucible (cathode) with internal diameter 19 mm, closed by cover with hole diameter 6 mm. Electron-beam heater was situated under the crucible. This heater could change the crucible temperature at the fixed current of arc. The water-cooled steel disc with central hole 15 mm in diameter was used as the anode.

At the temperature 1.25 kK which corresponds to plumbum saturated vapor pressure about 0.1 kPa voltage from power source (380 V, 200 A) was applied to anode and high-voltage discharge initiated with characteristics mentioned above. After a few seconds this discharge could turn into arc, or could exist hundreds of seconds until full plumbum evaporation. Crucible temperature increase until 1.4 kK accompanied by rising of plasma radiation intensity but under these conditions high-voltage discharge didn't switch to arc regime. At the temperature of 1.15 kK the discharge spontaneously disappeared. At more high temperatures discharge may also spontaneously fade but then it ignites again.

The pictures of discharge glow are described. They could take the form of a cone, harness, or plasma bunch, which is at the appreciable distance from the electrodes. The estimations of plasma parameters are presented.

The study was supported by grant from the Russian Scientific Fund (project #14-29-00231).

PRODUCTION AND STUDY OF MEGAWATT AIR–NITROGEN PLASMATRON WITH DIVERGENT CHANNEL OF OUTPUT ELECTRODE

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In recent years great interest in science world is caused by megawatt plasmatrons which produce high-enthalpy plasma streams with large diameter for use in plasma-chemical technologies. The interest is due to the fact that it is possible to obtain extremely high temperatures which are unattainable by chemical methods, reliability, compact size, on demand start and stop of operation mode and easy way to control the power output of plasmatron. Plasmatron generates a megawatt high-enthalpy plasma jet ($H \geq 30$ kJ/g), it belongs to the class of plasmatrons with thermionic cathode, tangential swirl flow and divergent channel output electrode-anode. Air–nitrogen plasmatron with power output of 1 MW using the original design of the main elements: cathode, gas flow rotation system and the anode can provide high flow performance when working on air and ensures the formation of slightly divergent ($2\alpha = 120$) air plasma jet with the diameter of $D = 50$ mm and mean plasma temperature of 6000–9000 K. To correctly register and study the parameters of plasma the experimental setup is equipped with seven diagnostic insertion holes to allow for the registration of the emission spectra across the cross section of the plasma stream at the outlet of plasmatron. Preliminary analysis of the obtained air plasma spectra shows that at a current of 1500 A near-axis zone of the plasma jet is characterized by a temperature of up to 15000 K, and the peripheral emission area has a temperature of 8000–9000 K. The electron temperature was determined by the relative intensities of the spectral lines N I and O I with different excitation energies of the upper levels. In the peripheral regions of the plasma jet multiple lines of Cu I (wall material of the plasma torch) in 400–525 nm region can be used to assess the plasma jet, Cu I spectral lines cover a wide range of excitation energies of 3.82–8.00 eV. The electron density of the air plasma is measured by the Stark component of the Voigt contour of lines $H\alpha$ (linear Stark effect) and atomic line O I 725.4 nm (quadratic Stark effect). In the axial region of a megawatt plasma stream the electron density is $(3 \pm 1) \cdot 10^{16}$ cm^{-3}.

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